# Tools for High Energy Physics Computations

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# Chapter 1

# Introduction

A great achievement of theoretical physics is the standard model of particle physics (hereafter SM). It unifies in the same framework the weak, electromagnetic and strong forces. Its predictions follow from a very restricted set of assumptions and a small number of fundamental constants that have to be determined experimentally.

Despite its simplicity, the SM has been proven to be in very good agreement with almost all experimental data accumulated in the last 50 years.

There are however indications that the SM does not describe the physics of energies above a few TeV, but is only a low energy effective theory of a more general theory. The SM in its minimal form fails to explain the observed neutrino mass and mixings. Another weak point of the SM is the so-called Higgs mass fine-tuning problem. The radiative corrections to the mass of the Higgs boson are quadratic, so that to avoid divergences, one has to fix the actual value of the Higgs mass to a precision of one in $10^{30}$. This procedure seems unnatural. The theorists also wish to unify gravitation (which is not a part of the SM) with the existing high energy model. In that respect, extensions of the SM which offers the possibility of including gravity in their framework are very attractive.

Due to the lack of experimental data in the range of energies where the SM is expected to fail, a wide choice of extensions of the SM have been proposed. Among the possibilities of extending the standard model, there is Supersymmetry which proposes a symmetry relating fermions with bosons. The presence of this symmetry forces the inclusion of partner particles, so called supersymmetric partners for each currently known particles, whose masses are above the energy reach of the current experiments.

One nice feature of supersymmetry is that it allows one to unify all forces at energy scales (a little bit lower than) the Plank scale. Another possibility is to enlarge the number of dimensions of the physical space, but to keep our low energy world in a 4 dimensional subspace.

The next challenge for high energy physics (and for the SM) will be the LHC, the Large Hadron Collider currently in construction at CERN. Since almost all the extensions of the SM introduce new particle at the TeV scale, the LHC offers the possibility of discriminating between these models.

## 1.1 The Standard model of particle physics

The SM of particle physics describes the known particles and their interaction. It encompasses the weak, electromagnetic and strong interactions.

The interaction between the matter particles is carried by bosonic particles of spin one. The photon is the carrier of the electromagnetic force, the $W$ and $Z$ boson are the carriers of the weak interaction, responsible for the beta decay of atoms. The strong force that glues the nucleus together is carried by the gluon.

Matter particles are fermions with spin one half. The matter particles are of two types, the quarks and the leptons. The leptons do not take part in the strong interaction, but only in the electroweak interaction. The quarks are the constituents of the nucleus. The leptons and quarks occur in a three-fold degeneracy, that is, for each lepton or quark there are two particles with exactely the same quantum numbers, except for the mass. The three different classes of particles are called generations. The SM is based on gauge theories. In these theories, the interactions are the consequence of the symmetry between particles. The symmetry group of the SM is $SU_3 \times SU_2 \times U_1$ The $SU_3$ colour symmetry is unbroken. The $SU_2 \times U_1$ are spontaneously broken, which leads to the mass of the weak gauge bosons $W$ and $Z$.

### 1.1.1 QCD

In this thesis, we are mainly interested in the part of the SM governed by the strong interaction. The theory describing the strong interaction is Quantum Chromo Dynamics (QCD). In this theory, the strong interaction between the quarks is carried by massless gluons. The charge of the quarks is called the colour. The gluon also carry a (colour) charge, unlike the photon that does not have a (electric) charge. One paradigm of QCD is so-called colour confinement, which states that at macroscopic scales, only colour neutral objects (e.g. no quarks or gluons) can be observed.

#### QCD factorization

One particularity of the strong interaction is the so called asymptotic freedom, which means that the strength of the interaction decreases with increasing energy. This allows us to treat QCD in perturbative theory, if the momentum transfer is high enough.

To study the properties of colour-charged objects, one has to collide colour neutral compound particles build up from colour-charged particles (hadrons).

Due to asymptotic freedom, the constituents of the hadrons (the partons) can be considered as free particles if the energy is large enough. The description of hadronic collision within the pQCD framework is obtained as follows. One first computes the cross section for the interaction between all combinations of colour-charged partons (the partonic cross sections), where the colour-charged particles are considered as free particles, then one convolves these partonic cross sections with the probability of finding the initial state colored particles in the hadrons. These probabilities are called parton density functions (PDFs). They are specific to the type of hadron but independent of the process considered, and can therefore be extracted from experimental data and used to make predictions for other experiments.

The final state particles can also carry a colour charge. Since no colour-charged particles can be observed as free state, the colour-charged particles will convert into colour-neutral particles. The experimental signature of a colour-charged particle is a more-or-less collimated bunch of particles called a jet. From characteristics of the jets one could infer information on the parton that produced it, without knowing the details of the particles forming the jets.

The conversion of partons into colour-neutral compound particles can be modeled in the form of so-called fragmentation functions which are the probability of a given final state parton to fragment into a given observed final state. In this case, to get a prediction for the experimental signature of the considered event, one has to convolve the result of the convolution of PDFs-partonic cross sections with these fragmentation functions.

## 1.2 Radiative corrections

The success of the physics program at LHC does not only rely on the experimental setup of the machine but also on the precise knowledge of the expected cross sections in the SM and its different extentions. Not only the cross sections of the process related to the expected new physics have to be computed, but also the cross sections of all processes of the SM which have the same or similar experimental signatures, the so-called background. A precise knowledge of the background is mandatory to separate effects of “known (boring)” SM physics from the “new (interesting!)” physics. It is not unusual that the extraction of this background from experimental data has to be carried out using theoretical predictions.

A precise prediction of the cross section for the production of new particles and their related background processes can be achieved using the framework of Quantum Field Theory (QFT) which provides a perturbative expansion in a small parameter of the cross sections of interest. In the case of the LHC, the underlying theory is perturbative Quantum Chromo Dynamics (pQCD). The cross section and other observables are computed as a series expansion in the strong coupling constant. At energies available at LHC, the strong coupling constant is of the order of 1/10, this means that the first term in this expansion, called Leading Order (LO), does not, in general, suffice to make a reliable prediction. The second term of the expansion, the so called Next-to-Leading Order (NLO) and sometimes also the third term, called Next-to-Next-to Leading Order (NNLO) have to be added to increase the reliability of the prediction.

The computation of an observable is thus composed of its LO contribution corrected by additional terms called radiative corrections. The computation of these additional terms is of increasing difficulty. For the corrections to a single given process there are more subprocesses to consider which are more difficult to compute than the original process. The main source of complication is the emergence of divergences, which will in the end cancel if the computation is done consistently, but these divergences prevent the direct numerical evaluation of the correction term. One has to first perform analytical work on the complicated expressions, in order to extract the singular behavior of the corrections, before evaluating the correction numerically.

### 1.2.1 Singularity structure of cross sections

The radiative corrections to a given process are composed of two different parts, the real and the virtual part that can (and have to) be computed separately. Both parts will have divergences but the sum of the two contributions yields a finite result. This cancellation is only possible if the divergent contributions of both the real and the virtual corrections are extracted on a consistent way. To achieve this goal, the two types of (divergent) corrections have to be regularized. The divergences are avoided by introducing a (more or less) unphysical parameter $\Lambda$. By taking this parameter to go to the physical limits we recover the physical result (and the divergences). This procedure is carried out on both corrections with the same regularization scheme so that the physical limit can be taken on the sum of the corrections and yield a well defined finite result, since the cancellation of the divergences is now apparent and parameterized by the parameter $\lambda$.

The most usual way to regularize the divergences in Yang-Mills theories is dimensional regularization, where the number of space-time dimensions $d = 4-2\epsilon$ is kept arbitrary. In this way, the divergences are displayed as poles in $\epsilon$, allowing for their explicit cancellation. Physical results are recovered by taking the limit $\epsilon \to 0$ after cancellation of the divergences. Another regularization scheme is the so called cut-off regularization where one eliminates the divergence due to large momenta in the loop momentum integrals by imposing a upper bound $\Lambda$ on the momentum integral. The divergences will be reduced to logarithms of ratios of the cutoff $\Lambda$ with scales present in the problem. These logarithms will cancel in the sum of the corrections, giving the expected finite result. Infrared divergences can be regularized by introducing a small mass parameter for massless particles like the photon or the gluon. This however violates gauge symmetry.

The necessity for radiative corrections is due to our inability to capture experimentally all the details of the interaction. Since we are unable to look directly in the interaction region but only observe asymptotic states far away from the interaction region, we can not distinguish events where no quantum fluctuations occurred from those where one (or more) occurred. On the other hand, in a realistic experiment, the granularity (the limit on the precision) of the detector(s) does not allow to distinguish between a process and the same process with one more particles emitted either with very small energy (soft) or in the same direction (collinear) as the primary particles. These two sorts of processes give rise to the same experimental signatures as the original process and contribute to the total experimentally-measured cross sections and have therefore to be taken into account in the theoretical prediction.

### Virtual corrections

The first contribution to the radiative corrections to a given process arises from quantum corrections in the form of internal off-shell particles propagating in a virtual loop. To compute the amplitude of this process, one has to integrate over the momenta of the internal particles. This integral can become divergent in two different ways.

First it can become divergent in the limit of very large internal momenta (so-called ultraviolet divergences), in which case a sensible result for the cross section is obtained by a redefinition of the a priori unphysical parameters of the Lagrangian. These parameters in the lagrangian have no physical meaning, before they are related through a prediction to experimental data. Given the measurement of some observable, one can infer the values for the parameters in the Lagrangian. From these values one can then make prediction for other processes. When dealing with UV divergences, the parameters of the Lagrangian are consistently set in such a way that the divergences cancel for every prediction.

The procedure of resetting the values of the parameters of the Lagrangian is called renormalization. The parameters of the Lagrangian are renormalized to match the physical data at a given scale. Doing it at another scale would lead to another numerical value for the parameters. The value of a physical observable does not depend on the place where we decide to match the parameters of the Lagrangian. When computing predictions with perturbation theory, the independence of the result from the renormalization scale is however not given any more. Since it would be, if one were to compute all orders in the perturbative series, one can use the dependence on the renormalization scale to estimate the error made by neglecting higher-order terms in the perturbation series.

The integral over the internal momenta can also become divergent in the case of massless internal particles for very small momenta. This divergence will eventually cancel with the infrared divergence of the real part of the NLO correction.

The standard method for dealing with virtual corrections is the Passarino-

Veltman reduction [1] which reduces the set of integrals arising from the loop momenta to scalar integrals. These are in turn reduced using integration by part identities to linear combinations of a much smaller set of basis integrals called master integrals, which are the only ones to be evaluated explicitly .

#### Real corrections

The second type of contributions to the radiative corrections to a given process is caused by the emission of one or more additional soft or collinear particles with the same initial state. The computation of this part of the radiative corrections requires the knowledge of the matrix elements of the process with more external particles (that can possibly become collinear or soft). These matrix elements will become divergent when the additional particles become collinear or soft with respect to one of the external particles.

The standard method for the computation of real corrections is the so-called subtraction method. The extraction of the divergent part is achieved by adding and subtracting a so-called subtraction term to the matrix element of the process with more final state partons. This subtraction term is designed to contain exactly the same divergences as the matrix element itself, being however simple enough to be integrated analytically over the phase space configuration where one or more particles become soft or collinear. The difference between the matrix element and the subtraction term is free of divergences and can (in principle) be integrated numerically. The art consists in the proper construction of subtraction terms. Catani and Seymour provided a general very algorithmic method for the construction of subtraction terms called dipole formalism [2]. Variations of this method have been proposed; one of them will be described in chapter 5.

### 1.2.2 Importance of radiative corrections

Due to the renormalization-scale dependence of the coupling strength, leading order predictions suffer from a large absolute normalization uncertainty. The inclusion of NLO is mandatory to reduce the normalization uncertainty of the LO order, as most NLO predictions have a preferred scale which reduces the scale uncertainties considerably. In addition NLO corrections may substantially change the kinematical shape of certain observables, such as the transverse jet-energy distribution. Therefore any precise measurements of the experiments at a hadron collider should be compared to theoretical predictions of at least NLO accuracy.

## 1.3 Outline

This thesis is divided into two parts. The first will present tools for high energy computations while the second shows some of their applications.

Due to the appearance of divergences in the radiative corrections to the cross section of high energy process, a straightforward numerical treatment is not possible. First some analytical work has to be done to extract the divergences from the correction, so that, once these divergences have been removed, the corrections can be computed numerically. One of these analytical tasks is to integrate complicated functions with arguments depending on the number of space-time dimensions $d$, which has to be kept arbitrary in the framework of dimensional regularization. In this context, hypergeometric functions and their generalizations are ubiquitous. The physical results are obtained by taking the limit where the arbitrary parameter $d$ goes to the physical four space-time dimensions. Thus it is not the exact result in $d$ but its expansion around $d = 4$ that is relevant for the purpose of computing physical quantities. Since $d$ often appears in the parameters of the hypergeometric functions, we are often confronted with the task of expanding these functions around given values of their parameters. Chapter 3 describes algorithms that allow to perform this expansion and present their implementation in a user-friendly tool.

The functions resulting from this expansion are called harmonic polylogarithms and have been introduced in ref. [3]. They are described in chapter 2, where we also present their extension to complex arguments. The implementation of their properties for the computer algebra program Mathematica is also presented.

Applications for the expansion of hypergeometric functions and the harmonic polylogarithms are presented in chapter 6, where hypergeometric functions are the result of the integration of master integrals. These have to be expanded around $d = 4$, which leads to expressions containing harmonic polylogarithms.

Chapter 5 is devoted to the extension of the antenna formalism [4–6] for the construction of infrared subtraction terms to processes with initial state partons, like for example at the LHC. An application of this extension is presented in chapter 7, where we construct the quark-quark induced contribution to the NNLO real correction to top pair production.

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# Part I

# Tools

# Chapter 2

# Harmonic polylogarithms

*This chapter is partly based on the paper*

*"HPL, a Mathematica implementation of the Harmonic Polylogarithms" [1] published with Tobias Huber in Computer Physics Communications.*

## 2.1 Introduction

Harmonic polylogarithms (HPLs) [2] are a generalization of the usual polylogarithms [3] and of the Nielsen polylogarithms [4]. HPLs appear in many calculations in high energy physics. Due to their construction through iterated integrations, they are useful for constructing solutions of differential equations, as they appear in the computation of master integrals. They are found in three-loop deeply inelastic splitting and coefficient functions [5–8], in two-loop massive vertex form factors [9–16], in two-loop Bhabha scattering [17–22], in multi-loop three-point and four-point functions [23–33] and 3-loop QED muon g-2 [34] and in more formal developments [35].

HPLs can be extended to complex arguments, like in two-loop massive master integrals [36, 37] and in the anomaly contribution to the heavy quark form factors [14].

HPLs of real arguments also show up the expansion of hypergeometric functions around their parameters for integer-valued parameters [38–41], whereas HPLs of imaginary arguments appear in the expansion of hypergeometric functions around half-integer parameters[1].

The HPLs have already been implemented for the algebraic manipulation language FORM [42]. This implementation is described in ref. [43] and can be found in ref. [44]. FORTRAN code for the numerical evaluation of the HPLs is also available [45]. A numerical implementation is also available for the C++ libraries GiNaC [46], described in ref. [47].

[1] see chapter 3

This chapter first reviews the properties of the HPLs described in ref. [2]. A new representation more suitable for the extension of the HPL to the complex plane is also presented. Then we present the `Mathematica` package `HPL` which provides an implementation of the properties presented in the first part, along with a numerical evaluation over the entire complex plane.

## 2.2 Properties of the harmonic polylogarithms

In this section, we review the properties of the HPLs described in ref. [2] that are covered by the implementation `HPL`. We also introduce a new representation that is more suitable for the extension of the HPLs to the complex plane.

Harmonic polylogarithms (HPL) are defined [2] through recursive integration of so-called weight functions. The number of integrations is called the weight of the HPL. The usual weights are

$$\begin{aligned} f_1(x) &= \frac{1}{1-x}\,, \\ f_0(x) &= \frac{1}{x}\,, \\ f_{-1}(x) &= \frac{1}{1+x}\,, \end{aligned} \tag{2.1}$$

and the corresponding weight-one HPLs are

$$\begin{aligned} H(1;x) &= \int_0^x f_1(t)\mathrm{d}t = \int_0^x \frac{1}{1-t}\mathrm{d}t = -\log(1-x), \\ H(0;x) &= \log(x)\,, \\ H(-1;x) &= \int_0^x f_{-1}(t)\mathrm{d}t = \int_0^x \frac{1}{1+t}\mathrm{d}t = \log(1+x)\,. \end{aligned} \tag{2.2}$$

HPLs of higher weights are then given by

$$\begin{aligned} H({}^n0;x) &= \frac{1}{n!}\log^n x\,, \\ H(a,a_{1,\ldots,k};x) &= \int_0^x f_a(t)H(a_{1,\ldots,k};t)\mathrm{d}t\,, \end{aligned} \tag{2.3}$$

where we use the notations

$${}^n i = \underbrace{i,\ldots,i}_{n} \quad \text{and} \quad a_{1,\ldots,k} = a_1,\ldots,a_k.$$

A useful notation introduced in ref. [2] for harmonic polylogs with non-zero rightmost index is given by dropping the zeros in the vector $a$, and adding 1 to the absolute value of the next non-zero index to the right for each dropped 0. This gives for example $(3,-2)$ for $(0,0,1,0,-1)$. We can extend this notation to all index vectors by allowing zeros to take place in the rightmost position of the new index vector. This gives for example $(3,-2,0,0)$ for $(0,0,1,0,-1,0,0)$. We will enclose index vectors in this notation in curly brackets and refer to it as the "m"-notation, as opposed to the "a"-notation. Some formulae or transformations are more easily expressed in the one or the other notation, therefore we keep both notations in parallel.

For the extension to arguments in the complex plane it is convenient to define the linear combinations

$$\begin{aligned} H(+;x) &= H(1;x) + H(-1;x) \;, \\ H(-;x) &= H(1;x) - H(-1;x) \;, \\ H(\pm, a_{1,\ldots,k};x) &= H(1, a_{1,\ldots,k};t) \pm H(-1, a_{1,\ldots,k};t) \;, \end{aligned} \tag{2.4}$$

which correspond to introducing the weight functions

$$f_+(x) = \frac{2}{1-x^2} \;, \qquad f_-(x) = \frac{2x}{1-x^2} \;. \tag{2.5}$$

We will refer to these two weights together with the weight $f_0$ as the "$\pm$" weights as opposed to the "integer" weights $f_1$, $f_0$ and $f_{-1}$.

The formula for the derivative of the HPLs follows directly from the definition

$$\frac{\mathrm{d}}{\mathrm{d}x} H(a, a_{1,\ldots,k};x) = f_a(x) H(a_{1,\ldots,k};x). \tag{2.6}$$

### 2.2.1 Product algebra

The product of two HPLs of weights $w_1$ and $w_2$ can be expressed as a linear combination of HPLs of weight $w = w_1 + w_2$. The formula in the "a"-notation for two HPLs with weight vectors $\mathbf{p}$ and $\mathbf{q}$ is given by

$$H(p_1,\ldots,p_{w_1};x) H(q_1,\ldots,q_{w_2};x) = H(\mathbf{p};x) H(\mathbf{q};x) = \sum_{r \in \mathbf{p} \uplus \mathbf{q}} H(\mathbf{r};x) \;, \tag{2.7}$$

where $\mathbf{p} \uplus \mathbf{q}$ is the set of all arrangements of the elements of $\mathbf{p}$ and $\mathbf{q}$ such that the internal order of the elements of $\mathbf{p}$ and $\mathbf{q}$ is kept. For example one has for $\mathbf{p} = (a,b)$ and $\mathbf{q} = (y,z)$

$$\begin{aligned} H(a,b;x)H(y,z;x) &= H(a,b,y,z;x) + H(a,y,b,z;x) \\ &\quad + H(a,y,z,b;x) + H(y,a,b,z;x) \\ &\quad + H(y,a,z,b;x) + H(y,z,a,b;x) \;. \end{aligned} \tag{2.8}$$

The product identity of the HPLs (2.7) is based on the general property

$$\int_0^t dx_1 \int_0^t dx_2 = \int_0^t dx_1 \int_0^{x_1} dx_2 + \int_0^t dx_2 \int_0^{x_2} dx_1 \ , \tag{2.9}$$

and is independent of the type of weights considered.

### 2.2.2 Extraction of the singular behavior

HPLs can have divergences in $x = 0$ and $x = 1$. The divergent part can be extracted with the help of the above product rules. Divergences at 0 are logarithmic with behavior $\simeq \log^n(x)$ if there are $n$ 0s at the right end of the index vector. In this case one can make the divergent behavior explicit by writing

$$\begin{aligned} & H(a_{1,\dots,k}; x) H(0; x) = \\ & \qquad H(a_{1,\dots,k}, 0; x) + H(a_{1,\dots,k-1}, 0, a_k; x) + \cdots + H(0, a_{1,\dots,k}; x) \ , \end{aligned} \tag{2.10}$$

which one can solve for $H(a_{1,\dots,k}, 0; x)$. Recalling that $H(0; x) = \log(x)$, the divergent log stands now explicitly outside the HPL. If there are more zeros in the right end of the index vector, one has to use this method recursively, until all trailing zeros have been exchanged for logs.

Similarly, when there are $n$ 1s or $-1$s at the very left of the index vector a logarithmic divergence $\simeq \log^n(1 \mp x)$ appears. It can be extracted in the same way as above. One cannot however extract simultaneously the $H(-1; x)$ and $H(1; x)$ divergent parts, as shown by the following example

$$H(1, -1; x) = H(-1; x) H(1; x) - H(-1, 1; x).$$

Since HPLs with $\pm$ weights contain singularities both at 1 and $-1$ it is only meaningful to extract the 0s from the weight vector.

### 2.2.3 Minimal set

The procedure for extracting the divergent parts of an HPL described in Section 2.2.2 allows to express many HPLs in terms of HPLs without divergences at 0 and 1 (so called "irreducible" ones) and products of HPLs of smaller weight. The product rules described in Section 2.2.1 also provide relations between HPLs of a given weight and HPLs of lower weight. One can combine all these relations to get a minimal set of HPLs for a given weight from which one can construct all other HPLs of this given weight, up to products of HPLs of lower weight. Table 2.1 shows the number of HPLs, irreducible HPLs and the dimension of the minimal set as a function of the weight [2].

Only the number of elements in the minimal set is fixed, there is a freedom left

| Weight | Full basis | Irreducible set | Minimal set |
|---|---|---|---|
| 1 | 3 | 3 | 3 |
| 2 | 9 | 4 | 3 |
| 3 | 27 | 12 | 8 |
| 4 | 81 | 36 | 18 |
| 5 | 243 | 108 | 48 |
| 6 | 729 | 324 | 116 |
| 7 | 2187 | 972 | 312 |
| 8 | 6561 | 2916 | 810 |

Table 2.1: Dimensions of the different bases

for the choice of which elements are to be taken as independent. Our choice was first to exclude all HPLs whose divergent behavior can be extracted along the lines of Section 2.2.2 from the minimal set. For the remaining ones, we ordered the index vectors with the following procedure. One adds one to all indices of the index vector (in the "a"-notation), the result is to be interpreted as the expansion in base 3 of a number. This number describes the index vector on a unique way. We used this numbering to sort the irreducible HPLs and choose to express later ones in terms of earlier ones.

As a consequence of the fact that the product identities rely on the general property (2.9) and not on the special form of the weight function, the reduction to a minimal set for HPLs of $\pm$ weights is exactly equivalent to the reduction to the minimal set for integer weights. In our implementation of the new $+-$ weights, we use exactly the same procedure as for the integer weights, replacing the weight $+1$ by $+$ and $-1$ by $-$.

### 2.2.4 Series expansion

In this section, we address the series expansion of the HPLs about $x = 0$. The HPLs are analytic in zero and can be expanded in a power series when the trailing zeros in the index vector are removed and expressed as logarithms. The series coefficients can be defined recursively. Let us call $Z_i(a_{1,\ldots,k})$ the coefficients of the expansion of $H\left(a_{1,\ldots,k}; x\right)$

$$H(a_{1,\ldots,k}; x) = \sum_{i=0}^{\infty} x^i Z_i(a_{1,\ldots,k}), \qquad Z_k(\ldots) = 0 \text{ for } k \leq 0\ . \tag{2.11}$$

We assume that the index vector has no trailing 0, as these lead to $\log(x)$ divergences. These divergences have to be made explicit by the procedure of Section 2.2.2. One can construct the coefficients $Z_i(a_{1,\ldots,k})$ recursively using the definition of the HPLs for $k > 1$

$$H(a, a_{1,\ldots,k}; x) = \int_0^x \mathrm{d}x' f_a(x') H(a_{1,\ldots,k}; x') = \sum_{i=0}^{\infty} Z_i(a_{1,\ldots,k}) \int_0^x \mathrm{d}x' f_a(x') x'^i . \tag{2.12}$$

For the three different possibilities $1, 0, -1$ for $a$ we get

$$\begin{aligned}
\int_0^x \frac{\mathrm{d}x'}{1-x'} x'^i &= \int_0^x \mathrm{d}x' \sum_{j=i}^{\infty} x'^j = \sum_{j=i+1}^{\infty} \frac{x^j}{j} , \\
\int_0^x \frac{\mathrm{d}x'}{x'} x'^i &= \frac{x^i}{i} , \\
\int_0^x \frac{\mathrm{d}x'}{1+x'} x'^i &= \int_0^x \mathrm{d}x' (x')^i \left( \sum_{j=0}^{\infty} (-x)^j \right) = (-1)^{i+1} \sum_{j=i+1}^{\infty} \frac{(-x)^j}{j} .
\end{aligned} \tag{2.13}$$

The recursion relation for the $Z_i$'s is found by interchanging the order of the summations over $i$ and $j$

$$\begin{aligned}
Z_j(1, a_{1,\ldots,k}) &= \frac{1}{j} \sum_{i=2}^{j} Z_{i-1}(a_{1,\ldots,k}) , \\
Z_j(0, a_{1,\ldots,k}) &= \frac{1}{j} Z_j(a_{1,\ldots,k}) , \\
Z_j(-1, a_{1,\ldots,k}) &= \frac{(-1)^j}{j} \sum_{i=2}^{j} (-1)^i Z_{i-1}(a_{1,\ldots,k}) .
\end{aligned} \tag{2.14}$$

For the "m"-notation, we can use the same notation for the coefficient of the series expansion, as no confusion is possible

$$H(\{m_{1,\ldots,k}\}; x) = \sum_{j=0}^{\infty} x^i Z_j(m_{1,\ldots,k}) .$$

Here again we assume that all $\log(x)$ divergences have been made explicit by the procedure of Section 2.2.2, so that the vector $m_{1,\ldots,k}$ has no trailing 0. The recursion relations for $n$ positive reads

$$\begin{aligned}
Z_j(n, m_{1,\ldots,k}) &= \frac{1}{j^n} \sum_{i=2}^{j} Z_{i-1}(m_{1,\ldots,k}) , \\
Z_j(-n, m_{1,\ldots,k}) &= \frac{(-1)^j}{j^n} \sum_{i=2}^{j} (-1)^i Z_{i-1}(m_{1,\ldots,k}).
\end{aligned} \tag{2.15}$$

The end points of the recursion are the expansions of $H(\{n\};x)$ and $H(\{-n\};x)$

$$\begin{aligned} H(\{n\};x) &= Li_n(x) = \sum_{i=1}^{\infty} \frac{x^i}{i^n} \ , \\ H(\{-n\};x) &= -Li_n(-x) = \sum_{i=1}^{\infty} \frac{-(-x)^i}{i^n} \ , \end{aligned} \tag{2.16}$$

which give

$$Z_i(\{n\}) = \begin{cases} \dfrac{\mathrm{sgn}(n)^{i+1}}{i^{|n|}} & i > 0 \\ 0 & i \leq 0 \ . \end{cases}$$

The coefficients for the series expansion of the $\pm$ weights can be found by adding or subtracting those for the integer weights, namely

$$\begin{aligned} Z_j(+,a_{1,\ldots,k}) &= \frac{1}{j}\sum_{i=2}^{j}(1+(-1)^{i+j})Z_{i-1}(a_{1,\ldots,k}) \\ Z_j(-,a_{1,\ldots,k}) &= \frac{1}{j}\sum_{i=2}^{j}(1-(-1)^{i+j})Z_{i-1}(a_{1,\ldots,k}) \ . \end{aligned} \tag{2.17}$$

### 2.2.5 Analytical properties

HPLs of integer weights have logarithmic divergences at $1, -1$ and branch cuts on $(-\infty,-1)$, $(1,\infty)$ or both depending on whether they have 1 or $-1$ weights occurring in their index vectors. HPLs with $\pm$ weights always have both branch cuts and have as many logarithmic singularities in both $-1$ and 1 as there are $+$s or $-$s before the first zero from the left of the weight vector.

HPLs have logarithmic ($\log^n(0)$) divergences at 0 if they have $n$ 0s at the right of the weight vector. They also have a branch cut on $(-\infty, 0)$.

### 2.2.6 Argument transformation

This section presents the argument transformations for HPLs. We will take the argument to lie in the complex plane with the two cuts $C_- = (-\infty,-1)$ and $C_+ = (1,\infty)$. We will further denote the upper half complex plane by $\mathbb{C}_+$ and the lower complex plane by $\mathbb{C}_-$. We consider the real axis on these cuts only as the limit of a complex argument approaching the real axis. So a "real argument with infinitesimal small positive imaginary part" will be addressed in this section exactly the same way as a argument in the upper complex plane.

For HPLs on the real axis the argument transformations described in ref. [2] map the integration range to a range starting or ending at a point where a potential singularity lies. Therefore these transformations have to be applied to

HPLs put into a form where the potentially divergent parts are explicitly factored out in the form of HPLs of weight one, for which the analytic continuation is known.

Extending the HPLs to the complex plane allows to map the integration so that it avoids the divergent points for each HPL, without having to put them in a factored form. We will refer to the transformation involving a transformation of the integration path into the complex plane as "complex", as opposed to the "real" transformations where the integration path is only on the real axis. In analogy to the "real" transformation which introduced HPLs evaluated at unity, the "complex" transformations introduce HPLs evaluated at $i$ and $-i$.

### The transformation $x \to -x$

We first consider the transformation $x \to -x$. It takes an argument from $\mathbb{C}_+$ into $\mathbb{C}_-$ and conversely. Using the definition of the HPLs,

$$\int_0^{-x} \mathrm{d}x' f_a(x') H(..., x') = -\int_0^{x} \mathrm{d}y f_a(y) H(..., -y), \tag{2.18}$$

we see that the weight functions transform the following way

$$\begin{array}{lll} f_1(x') \to -f_{-1}(y) & f_0(x') \to f_0(y) & f_{-1}(x') \to -f_1(y) \\ f_+(x') \to -f_+(y) & & f_-(x') \to +f_-(y)\ . \end{array} \tag{2.19}$$

The transformation of HPLs without trailing 0's is easily done, we have for integer weights

$$H(n_1, ..., n_w; -x) = (-1)^s H(-n_1, ..., -n_w; x)\ , \tag{2.20}$$

with $s$ given by the number of non zero weights (the length of the vector in the "m" notation) and for $\pm$ weights by

$$H(s_1, ..., s_w; -x) = (-1)^s H(s_1, ..., s_w; x)\ , \tag{2.21}$$

with this time $s$ given by the number of + weights only. So we see that HPL with $\pm$ weights and no trailing zeros are either odd or even, when the number of + weights is odd or even, respectivly.

The case of trailing zeros is more tricky. Consider $x = re^{i\phi}$

$$H_0(x) = \log x = \log(r) + i\phi\ , \qquad H_0(-x) = \log(-x) = \log(r) + i(\phi \pm \pi)\ , \tag{2.22}$$

with the + sign for argument in $\mathbb{C}_-$ and $-$ for $\mathbb{C}_+$. HPLs of higher weights with trailing zeros can be treated by extracting the trailing zeros, as described in Section 2.2.2.

**The transformation $x \to 1/x$**

We consider the transformation
$$x = \frac{1}{y}$$
for HPLs with $\pm$ weights. The results for integer weights can be obtained in the same way and are described in refs. [1, 2]. The identities for weight 1 read

$$\begin{aligned} H(0;x) &= -H(0;y), \\ H(+;x) &= H(+;y) + i\pi\Theta(x), \\ H(-;x) &= H(-;y) + 2H(0;y) + i\pi\Theta(x). \end{aligned} \tag{2.23}$$

where $\Theta(x)$ is $+1$ in the upper half complex plane and $-1$ in the lower half complex plane. For higher weight we proceed by induction. We take $x$ to be in the lower complex plane, so that $y$ is in the upper complex plane. We split the integration into two pieces,

$$\begin{aligned} H(s, s_{2,\ldots,k}; y) &= \int\limits_0^{1/x} \mathrm{d}x' f_s(x') H(s_{2,\ldots,k}; t) = \left( \int\limits_0^{i} \mathrm{d}x' + \int\limits_i^{\frac{1}{x}} \mathrm{d}x' \right) f_s(x') H(s_{2,\ldots,k}; x') \\ &= H(s, s_{2,\ldots,k}; i) - \int\limits_{-i}^{x} \frac{\mathrm{d}t'}{t'^2} f_s\left(\frac{1}{t'}\right) H\left(s_{2,\ldots,k}; \frac{1}{t'}\right) \\ &= H(s, s_{2,\ldots,k}; i) - \left( \int\limits_0^{x} - \int\limits_0^{-i} \right) \frac{\mathrm{d}t'}{t'^2} f_s\left(\frac{1}{t'}\right) H\left(s_{2,\ldots,k}; \frac{1}{t'}\right) . \end{aligned} \tag{2.24}$$

We have for the different cases $s = 0$ and $s = +$ and $s = -$,

$$\begin{aligned} \frac{\mathrm{d}t}{t^2} f_0\left(\frac{1}{t}\right) &= \frac{\mathrm{d}t}{t}\mathrm{d}t = f_0(t)\mathrm{d}t\ , \\ \frac{\mathrm{d}t}{t^2} f_+\left(\frac{1}{t}\right) &= \mathrm{d}t\left(\frac{1}{t^2-1}\right) = -f_+(t)\mathrm{d}t\ , \\ \frac{\mathrm{d}t}{t^2} f_-\left(\frac{1}{t}\right) &= \mathrm{d}t\left(\frac{2}{(t^2-1)t}\right) = \mathrm{d}t\left(\frac{2t}{t^2-1} - \frac{2}{t}\right) = \left(-f_-(t) - 2f_0(t)\right)\mathrm{d}t. \end{aligned} \tag{2.25}$$

We only need to replace
$$H\left(s_{2,\ldots,k}; \frac{1}{t'}\right)$$
by its representation in terms of HPLs of argument $t'$. The case of $x$ in the lower complex plane is treated exactly on the same way, separating the integration at $x' = -i$.

**The transformation** $x \to \dfrac{1-x}{1+x}$

We consider the transformation

$$x = \frac{1-y}{1+y}$$

for HPLs with $\pm$ weights. The results for the integer weights obtained on the same way and are described in [1, 2]. The identities for weight 1 read

$$\begin{aligned} H(0;x) &= -H(+;y), \\ H(+;x) &= -H(0;y), \\ H(-;x) &= -H(0,y) + H(+,y) - H(-;y) - 2\log 2. \end{aligned} \tag{2.26}$$

For higher weight we proceed by induction. We split the integration into two pieces.

$$\begin{aligned} H(s,s_{2\ldots k};y) = \int\limits_0^{\frac{1-x}{1+x}} \mathrm{d}x' f_s(x') H(s_{2\ldots k};t) &= \left( \int\limits_0^{i} \mathrm{d}x' + \int\limits_i^{\frac{1-x}{1+x}} \mathrm{d}x' \right) f_s(x') H(s_{2,\ldots,k};x') \\ = \quad H(s,s_{2,\ldots,k};i) - \int\limits_{-i}^{x} \frac{2\mathrm{d}t'}{(1+t')^2} f_s\left(\frac{1-t'}{1+t'}\right) H\left(s_{2,\ldots,k};\frac{1-t'}{1+t'}\right) \\ = \quad H(s,s_{2,\ldots,k};i) - \left( \int\limits_0^{x} - \int\limits_0^{-i} \right) \frac{2\mathrm{d}t'}{(1+t')^2} f_s\left(\frac{1-t'}{1+t'}\right) H\left(s_{2,\ldots,k};\frac{1-t'}{1+t'}\right) \; . \end{aligned} \tag{2.27}$$

We have for the different cases $s=0$, $s=+$ and $s=-$,

$$\begin{aligned} \frac{2\mathrm{d}t'}{(1+t')^2} f_0\left(\frac{1-t'}{1+t'}\right) &= \frac{2\mathrm{d}t'}{1-t'^2} = f_+(t')\mathrm{d}t' \; , \\ \frac{2\mathrm{d}t'}{(1+t')^2} f_+\left(\frac{1-t'}{1+t'}\right) &= \frac{1}{t'}\mathrm{d}t' = f_0(t')\mathrm{d}t' \; , \\ \frac{2\mathrm{d}t'}{(1+t')^2} f_-\left(\frac{1-t'}{1+t'}\right) &= \mathrm{d}t' \frac{1-t'}{t'(1+t')} = \left(f_0(t') - f_+(t') + f_-(t')\right)\mathrm{d}t'. \end{aligned} \tag{2.28}$$

Now we only need to replace

$$H\left(s_{2,\ldots,k};\frac{1-t'}{1+t'}\right)$$

by its expansion in terms of HPLs of argument $t'$ and perform the integration using the definition of the HPLs.

### The transformation $x^2 \to x$

Since we cannot express $1+x^2$ as sum of the basis functions $f_1$, $f_0$ and $f_{-1}$, we will exclude index vectors with negative indices for our considerations. The identities for weight 1 are

$$\begin{aligned} H(0;x^2) &= \log(x^2) = 2H(0;x), \\ H(1;x^2) &= -\log(1-x^2) = H(1;x) - H(-1;x) = H(-;x). \end{aligned} \tag{2.29}$$

The first identity holds on the complex plane except for the branch cut $(-\infty,0)$ whereas the second equation holds on the entire complex plane except for $(1,\infty)$. For higher weights we use the relations,

$$\begin{aligned} H(0,m_{2\ldots,k};x^2) &= \int_0^{x^2} \frac{\mathrm{d}x'}{x'} H(m_{2,\ldots,k};x') \\ &= 2\int_0^{x} \frac{\mathrm{d}t'}{t'} H(m_{2,\ldots,k};t'^2), \\ H(1,m_{2\ldots,k};x^2) &= \int_0^{x^2} \frac{\mathrm{d}x'}{1-x'} H(m_{2,\ldots,k};x') \\ &= \int_0^{x} \mathrm{d}t' \left(\frac{1}{1-t'} - \frac{1}{1+t'}\right) H(m_{2,\ldots,k};t'^2) \end{aligned} \tag{2.30}$$

recursively, where $H(m_{2,\ldots,k};t'^2)$ is expressed as HPLs of argument $t'$, which are known in a recursive approach.

### The transformation $x \to 1-x$

We consider the transformation

$$x \to 1-x.$$

Since $1/(2-x)$ (the transform of $1/(1+x) = f_{-1}$) can not be expressed as linear combinations of the $f_i$'s, we will only consider index vectors without a negative index. We first have the identities for weight 1

$$\begin{aligned} H(0;1-x) &= \log(1-x) = -H(1;x), \\ H(1;1-x) &= -\log(x) = -H(0;x). \end{aligned} \tag{2.31}$$

Again, these identities hold everywhere except for $x$ in $(-\infty,0)$ or in $(1,\infty)$ . Here again, we evaluate recursively in the depth. We use the fact that one can express HPLs with 1s on the left of the index vector as product of $H(1;x)$ (whose transformation we know from above) and HPLs without left 1s and treat only the case of a 0 as the left index. For this we use the formula

$$\begin{aligned} H(0, m_{2\ldots,k}; 1-x) &= \int_0^{1-x} \frac{\mathrm{d}x'}{x'} H(m_{2,\ldots,k}; x') \\ &= \int_0^1 \frac{\mathrm{d}t'}{t'} H(m_{2,\ldots,k}; x') - \int_{1-x}^1 \frac{\mathrm{d}x'}{x'} H(m_{2,\ldots,k}; x') \\ &= H(0, m_{2,\ldots,k}; 1) - \int_0^x \frac{\mathrm{d}t'}{1-t'} H(m_{2,\ldots,k}; 1-t')\ , \end{aligned} \tag{2.32}$$

where one has to insert for $H(m_{2,\ldots,k}; 1-t')$ the expansion in terms of HPLs of argument $t'$ known from the recursion. The HPLs (with positive $m$s) evaluated for argument 1 are related to the multiple zeta values (MZV). This aspect is treated in Section 2.2.8.

### 2.2.7 HPLs on the imaginary axis

A nice property of the HPLs of weights + and − are that they are (provided they have no trailing zeros) either purely real or imaginary. Appending a + weight to an HPL that is real on the imaginary axis will change it into purely imaginary and vice versa. Appending a − weight doesn't change its nature.

### 2.2.8 Values at unity and multiple zeta values

HPLs of argument 1 are constants and deserve special treatment. They are related for positive $m$s to the Multiple Zeta Values (MZVs) and for general $m$s to colored MZVs. The relation can be found through induction and reads[2]

$$\begin{aligned} H(\{m_{1,\ldots,k}\}; 1) &= N(m_{1,\ldots,k})\zeta(\tilde{m}_{1,\ldots,k}), \quad k > 1\ , \\ H(\{m\}; 1) &= \zeta(m)\ , \qquad m > 0\ , \\ H(\{-m\}; 1) &= (1-2^{1-m})\zeta(m)\ , \qquad m > 0\ . \end{aligned} \tag{2.33}$$

The MZVs $\zeta$ are defined by,

$$\zeta(m_1, \ldots, m_k) = \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1-1} \cdots \sum_{i_k=1}^{i_{k-1}-1} \prod_{j=1}^{k} \frac{\mathrm{sgn}(m_j)^{i_j}}{i_j^{|m_j|}}\ , \tag{2.34}$$

and are described in the literature, for example in refs. [48, 49]. The vector $\tilde{m}$ is obtained from the vector $m$ via

$$\tilde{m} = (m_1, \mathrm{sgn}(m_1)m_2, \ldots, \mathrm{sgn}(m_{i-1})m_i, \ldots, \mathrm{sgn}(m_{k-1})m_k)\ . \tag{2.35}$$

[2]see appendix 2.C for a proof.

The factor $N(m_{1,\ldots,k})$ is given by

$$N(m_{1,\ldots,k}) = (-1)^{\#(m_i<0)} \ . \tag{2.36}$$

The MZV's also form an algebra. Due to this fact, they can be expressed in terms of a few mathematical constants like powers of $\pi$, $\zeta$-functions and polylogs at specified values. We list some of the identities of refs. [48, 49] in Appendix 2.A. For the implementation of the HPL at unity, we translated the tables of the FORM package `harmpol.h` [2] and their expansions for weight 7 and 8 `htable7.prc` and `htable8.prc` to Mathematica.

In these tables, there appear some constants that are not expressible through usual constants like $\pi$, $\zeta(n)$, $\log(2)$, or $Li_n(1/2)$. Using the different relations between the different MZVs, one can reduce the number of independent constants. These independent constants are listed in appendix 2.B.

For index vectors with left 1's, there appear divergences of the form

$$\sum_{i=1}^{\infty} \frac{1}{i} = S(1,\infty) = H(1;1).$$

These divergences are well defined[3] and can cancel during a calculation. Right 0s can be extracted with the method of Section 2.2.2. All factors $H(0;1) = \log(1) = 0$ vanish, even when multiplied by $H(1;1) = -\log(0)$, since

$$\log(x)\log^n(1-x) \to 0, \qquad x \to 0, \quad n > 0.$$

**Values at $i$**

The argument transformations of the above Section 2.2.6 use the values of the HPLs with $\pm$ weights at $x = i$. For the lower weights we have

$$\begin{aligned}
H(+,i) &= \frac{i\pi}{2} & H(-,i) &= \log(2)\ , \\
H(+,-,i) &= i\,(2\mathcal{C} - \pi\log(2))\ , & H(-,+,i) &= i\left(-2\mathcal{C} + \frac{1}{2}\pi\log(2)\right)\ , \\
H(0,+,i) &= 2i\mathcal{C}\ , & H(0,-,i) &= \frac{-\pi}{24}\ , \\
H(+,0,i) &= -2i\mathcal{C} - \frac{\pi^2}{4}\ , & H(-,0,i) &= \frac{-\pi}{24} - \frac{i}{2}\pi\log(2)\ ,
\end{aligned} \tag{2.37}$$

where $\mathcal{C}$ is Catalan's constant

$$\mathcal{C} = \sum_{k=0}^{\infty} \frac{1}{(2k+1)^2}\ .$$

To find the values at $i$ for higher weights, one can use the following properties

[3] see ref. [2] for more details.

- The product identities relates HPLs in $i$ with HPLs of lower weights at $i$.
- Some HPLs can be written in terms of more commonly known functions, whose values at $x = i$ are known.
- Using the argument transformation $x^2 \to x$ one can relate the values of HPLs with only "$-$" and 0 weights to the values of HPLs with integer weights at $-1$.
- Since the "complex" transformations of Section 2.2.6 involve HPLs at $i$ and the "real" ones not, comparing them leads to relations between different HPLs at $i$.

The number of relations is, however not sufficient to solve for all HPLs at $i$. A list of values of HPLs at $i$ is given in Appendix 2.E

## 2.3 The Mathematica implementation `HPL 2`

In this section, we describe the extension of the Mathematica implementation `HPL` to complex arguments. Version 2 of `HPL` includes all features of the first version as well as the following new elements,

- numerical evaluation of HPLs for complex arguments,
- new weights + and $-$,
- new function `HPLArgTransform`.

For completeness, we will not restrict the description to the new features of `HPL` but will also repeat the features that did not change. The package can be found at link [50] where installation instructions can be found. After installation, the package can be loaded via

```
<< HPL-2.0.m
```

It should be loaded at the beginning of the `Mathematica` session.

### 2.3.1 New functions

The package `HPL` defines the following new functions

- `HPL[m,x]` is the harmonic polylogarithm $H(m; x)$, where `m` is a list representing the index vector. For integer weights, we chose the "m"-notation as the standard notation. It is possible to give as the argument a vector in the "a"-notation, or even in a mix between the two notations, as no confusion is possible. Results will be displayed in the "m"-notation. It is also possible to mix $\pm$ and integer weights.

```
*********** HPL 2.0 **************
Author: Daniel Maitre, University of Zurich
Rules for minimal set loaded for weights: 2, 3, 4, 5, 6.
Rules for minimal set for + - weights loaded for weights: 2, 3, 4, 5, 6.
Table of MZVs loaded up to weight 6
Loading Tables of values at I loaded up to weight 6
Table of values at I loaded
HPL[{2, 1}, x]
HPL[{1, 0, -1}, x]
HPL[{plus, minus}, x]
HPL[{plus, 3, minus}, x]
HPL[{2, 1}, x]
HPL[{1, -2}, x]
HPL[{plus, minus}, x]
HPL[{plus, 3, minus}, x]
```

- `HPLMtoA[m_List]`,`HPLAtoM[a_List]` convert vectors from the "m"- to the "a"-, and from the "a"- to the "m"-notation respectively. Both can convert vectors which mix the two notations.

```
HPLMtoA[{2, -3, 0}]
HPLAtoM[{1, 0, 0, 1, 0, -1, 0}]
{0, 1, 0, 0, -1, 0}
{1, 3, -2, 0}
HPLMtoA[{2, plus, minus, 0}]
HPLAtoM[{0, 1, plus, 0, minus, 0}]
{0, 1, plus, minus, 0}
{2, plus, 0, minus, 0}
```

- `HPLpm21m1`, `HPL1m12pm` convert HPLs with $\pm$ weights into HPLs with integer weights and vice versa.

```
HPLpm21m1[HPL[{plus, minus}, t]]
-HPL[{-1, -1}, t] + HPL[{-1, 1}, t] - HPL[{1, -1}, t] + HPL[{1, 1}, t]
HPL1m12pm[HPL[{1, -2}, x]]
-1/4 HPL[{minus, 0, minus}, x] + 1/4 HPL[{minus, 0, plus}, x] -
 1/4 HPL[{plus, 0, minus}, x] + 1/4 HPL[{plus, 0, plus}, x]
```

It is also possible to convert a function with integer weights into the corresponding sum of functions of of $\pm$ weights, and vice versa.

```
HPLpm21m1[{plus, minus}, f]
-f[-1, -1] + f[-1, 1] - f[1, -1] + f[1, 1]
HPL1m12pm[{1, -2}, f]
-1/4 f[minus, 0, minus] + 1/4 f[minus, 0, plus] - 1/4 f[plus, 0, minus] + 1/4 f[plus, 0, plus]
```

- `HPLLogExtract` extracts the singular behavior of HPLs, using the methods presented in Section 2.2.2, for

  **integer weights** in their argument at 0 and 1.

  $+-$ **weights** in their argument only at 0.

  The result is displayed as function of $\log(x), \log(1-x)$ or $H(1;x), H(0;x)$ depending on the option settings (see Section 2.3.3).

```
HPLLogExtract[HPL[{1, 2}, x]]
HPL[{1}, x] HPL[{2}, x] - 2 HPL[{2, 1}, x]
HPLLogExtract[HPL[{plus, minus, 0}, x]]
HPL[{0}, x] HPL[{plus, minus}, x] - HPL[{0, plus, minus}, x] - HPL[{plus, 0, minus}, x]
$HPLAutoConvertToKnownFunctions = True;
HPLLogExtract[HPL[{1, 2}, x]]
-Log[1 - x] PolyLog[2, x] -
 2 (1/2 Log[1 - x]^2 Log[x] + Log[1 - x] PolyLog[2, 1 - x] - PolyLog[3, 1 - x] + Zeta[3])
HPLLogExtract[HPL[{plus, minus, 0}, x]]
-HPL[{0, plus, minus}, x] - HPL[{plus, 0, minus}, x] + HPL[{plus, minus}, x] Log[x]
```

  In the case of mixed integer and $\pm$ weights, only the divergences at 0 are factored.

- `HPLConvertToKnownFunctions` returns its argument with HPLs replaced by their representation in terms of more common functions, whenever possible.

```
HPLConvertToKnownFunctions[HPL[{2, 2}, x]]
1/2 PolyLog[2, x]^2 - 2 PolyLog[2, 2, x]
HPLConvertToKnownFunctions[HPL[{plus}, x]]
Log[(1 + x)/(1 - x)]
```

  It is only needed if the option `$HPLAutoConvertToKnownFunctions` is set to `False` (see Section 2.3.3).

- `HPLProductExpand` returns the value obtained by replacing products of HPLs of same argument by their representation as a linear combination of HPLs, as presented in Section 2.2.1.

```
HPLProductExpand[HPL[{2, 1}, t] HPL[{1, 0}, t]]
HPL[{1, 2, 2}, t] + 2 HPL[{1, 3, 1}, t] + 2 HPL[{2, 1, 2}, t] +
 HPL[{2, 2, 1}, t] + HPL[{1, 2, 1, 0}, t] + 3 HPL[{2, 1, 1, 0}, t]
HPLProductExpand[HPL[{1, 0}, t] HPL[{-1}, t] HPL[{1, -1}, t]]
2 HPL[{-1, 1, 1, -2}, t] + HPL[{-1, 1, 2, -1}, t] + HPL[{1, -2, 1, -1}, t] +
 3 HPL[{1, -1, 1, -2}, t] + HPL[{1, -1, 2, -1}, t] + 4 HPL[{1, 1, -2, -1}, t] +
 4 HPL[{1, 1, -1, -2}, t] + 2 HPL[{1, 2, -1, -1}, t] + HPL[{-1, 1, -1, 1, 0}, t] +
 2 HPL[{-1, 1, 1, -1, 0}, t] + 2 HPL[{1, -1, -1, 1, 0}, t] +
 3 HPL[{1, -1, 1, -1, 0}, t] + 4 HPL[{1, 1, -1, -1, 0}, t]
```

```
HPLProductExpand[HPL[{plus, minus}, t] HPL[{1, -1}, t]]
HPL[{1, -1, plus, minus}, t] + HPL[{1, plus, -1, minus}, t] + HPL[{1, plus, minus, -1}, t] +
 HPL[{plus, 1, -1, minus}, t] + HPL[{plus, 1, minus, -1}, t] + HPL[{plus, minus, 1, -1}, t]
```

In order to expand all products, `HPLProductExpand` expands its argument (using `Expand`), so that terms of the form

$$H(\dots;x)\big(H(\dots;x)+H(\dots;x)+\dots\big).$$

are also replaced. For large expressions this might be time consuming, one should in this case first collect the products of HPLs and apply `HPLProductExpand` only to the products and not to the whole expression.

```
HPLProductExpand[HPL[{2}, t] (HPL[{1, 0}, t] + HPL[{-1}, t])]
HPL[{-2, 1}, t] + HPL[{-1, 2}, t] + 2 HPL[{1, 3}, t] +
 HPL[{2, -1}, t] + HPL[{2, 2}, t] + HPL[{1, 2, 0}, t] + 2 HPL[{2, 1, 0}, t]
```

Since the product properties are general, the function works for any vectors of symbolic weights.

```
HPLProductExpand[HPL[{a, b}, x] HPL[{y, w, z}, x]]
HPL[{a, b, y, w, z}, x] + HPL[{a, y, b, w, z}, x] +
 HPL[{a, y, w, b, z}, x] + HPL[{a, y, w, z, b}, x] +
 HPL[{y, a, b, w, z}, x] + HPL[{y, a, w, b, z}, x] + HPL[{y, a, w, z, b}, x] +
 HPL[{y, w, a, b, z}, x] + HPL[{y, w, a, z, b}, x] + HPL[{y, w, z, a, b}, x]
```

- `HPLConvertToSimplerArgument` returns its argument with HPLs of related arguments replaced by their expansion as a sum of HPLs of simpler arguments. Which transformations are implemented depends on the type of weights. They are:

**integer weights** $-x$, $x^2$, $1-x$, $1/x$, $x/(x-1)$ and $(1-x)/(1+x)$

$\pm$ **weights** $-x$, $1/x$, and $(1-x)/(1+x)$.

```
HPLConvertToSimplerArgument[HPL[{2, 1}, -x]]
HPL[{-2, -1}, x]
HPLConvertToSimplerArgument[HPL[{2, 1}, 1 - x]]
-HPL[{1, 0, 0}, x] + Zeta[3]
HPLConvertToSimplerArgument[HPL[{1, 1}, (1 - x)/(1 + x)]]
1/2 (HPL[{-1}, x] - HPL[{0}, x] - Log[2])^2
HPLConvertToSimplerArgument[HPL[{2}, (x) / (x - 1)]]
-HPL[{2}, x] - HPL[{1, 1}, x]
HPLConvertToSimplerArgument[HPL[{plus, minus}, (1 - x) / (1 + x)]]
π^2/6 + HPL[{0, 0}, x] + HPL[{0, minus}, x] - HPL[{0, plus}, x] + 2 HPL[{0}, x] Log[2]
```

The transformations do not work for mixed integer and $\pm$ weights.

- `HPLArgTransform[x ,r ,δ ]` returns its first argument expressed in terms of HPLs of the transformed argument. It does the same job as `HPLConvertToSimplerArgument`
  , but the transformation to be performed is not fixed by the form of the argument of the HPL but is specified as an argument of `HPLArgTransform`.

```
HPLArgTransform[HPL[{2, -1}, X], x → -x]
HPLArgTransform[HPL[{plus, 0, minus}, X], x → -x]
HPL[{-2, 1}, -X]
-HPL[{plus, 0, minus}, -X]
```

`HPLArgTransform[HPL[{2, 1}, X], x → √x]`

$$2\left(\text{HPL}\left[\{-2,-1\},\sqrt{X}\right]-\text{HPL}\left[\{-2,1\},\sqrt{X}\right]-\text{HPL}\left[\{2,-1\},\sqrt{X}\right]+\text{HPL}\left[\{2,1\},\sqrt{X}\right]\right)$$

`HPLArgTransform[HPL[{1, 1, 2}, X], x → 1 - x]`

$$\frac{1}{2}\text{HPL}[\{0\},1-X]^2\left(\frac{\pi^2}{6}+\text{HPL}[\{1,0\},1-X]\right)+$$
$$3\left(\frac{\pi^4}{90}+\text{HPL}[\{1,0,0,0\},1-X]\right)+2\,\text{HPL}[\{0\},1-X]\,(-\text{HPL}[\{1,0,0\},1-X]+\text{Zeta}[3])$$

In addition one can specify whether the argument is assumed to lie in the upper ($\delta$=+1) or lower ($\delta = -1$) complex plane, or whether to leave it purely symbolic.

`HPLArgTransform[HPL[{2, 2}, X], x → x / (x - 1)]`

$$\text{HPL}\left[\{2,2\},\frac{X}{-1+X}\right]+\text{HPL}\left[\{1,1,2\},\frac{X}{-1+X}\right]+$$
$$\text{HPL}\left[\{2,1,1\},\frac{X}{-1+X}\right]+\text{HPL}\left[\{1,1,1,1\},\frac{X}{-1+X}\right]$$

`HPLArgTransform[HPL[{2}, X], x → (1 - x) / (1 + x), δ]`

$$\frac{\pi^2}{6}-\text{HPL}\left[\{-1,-1\},\frac{1-X}{1+X}\right]+\text{HPL}\left[\{-1,0\},\frac{1-X}{1+X}\right]-\text{HPL}\left[\{1,-1\},\frac{1-X}{1+X}\right]+$$
$$\text{HPL}\left[\{1,0\},\frac{1-X}{1+X}\right]+\text{HPL}\left[\{-1\},\frac{1-X}{1+X}\right]\text{Log}[2]+\text{HPL}\left[\{1\},\frac{1-X}{1+X}\right]\text{Log}[2]$$

`HPLArgTransform[HPL[{plus, 0, minus}, X], x → (1 - x) / (1 + x), δ]`

$$-\text{Catalan}\,\pi-\frac{i\,\pi^3}{24}-\frac{1}{12}\pi^2\,\text{HPL}\left[\{0\},\frac{1-X}{1+X}\right]-\text{HPL}\left[\{0,\text{plus},0\},\frac{1-X}{1+X}\right]-$$
$$\text{HPL}[\{0,\text{plus},\text{minus}\},i]-\text{HPL}\left[\{0,\text{plus},\text{minus}\},\frac{1-X}{1+X}\right]-\text{HPL}[\{0,\text{plus},\text{plus}\},i]+$$
$$\text{HPL}\left[\{0,\text{plus},\text{plus}\},\frac{1-X}{1+X}\right]+\text{HPL}[\{\text{plus},0,\text{minus}\},i]-4\,i\,\text{Catalan}\,\text{Log}[2]-$$
$$2\,\text{HPL}\left[\{0,\text{plus}\},\frac{1-X}{1+X}\right]\text{Log}[2]+\frac{1}{16}\,i\,\text{Zeta}\left[3,\frac{1}{4}\right]-\frac{1}{16}\,i\,\text{Zeta}\left[3,\frac{3}{4}\right]$$

`HPLArgTransform[HPL[{2, -2}, X], x → 1 / x, δ₁]`

$$\frac{37\,\pi^4}{720}+\text{HPL}[\{-4\},X]-\frac{1}{6}\pi^2\,\text{HPL}[\{2\},X]-\frac{1}{6}\pi^2\,\text{HPL}[\{0,0\},X]+$$
$$\text{HPL}[\{2,-2\},X]-\text{HPL}[\{2,0,0\},X]-\text{HPL}[\{0,0,0,0\},X]-$$
$$\frac{1}{12}\,i\,\pi^3\,\text{HPL}[\{0\},X]\,\delta_1+2\,\text{HPL}[\{0\},X]\left(\frac{1}{4}\pi^2\,\text{Log}[2]-\text{Zeta}[3]\right)+$$
$$\frac{1}{4}\text{HPL}[\{0\},X]\,\text{Zeta}[3]+2\,\text{HPL}[\{0\},X]\left(-\frac{1}{4}\pi^2\,\text{Log}[2]+\frac{13\,\text{Zeta}[3]}{8}\right)$$

```
HPLArgTransform[HPL[{minus, 0, plus}, X], x → 1 / x, δ2]
```

$$-2\,\mathrm{HPL}\left[\{0,0,\mathrm{plus}\},\frac{1}{X}\right]-\mathrm{HPL}\left[\{\mathrm{minus},0,\mathrm{plus}\},\frac{1}{X}\right]-\frac{5}{24}\,i\,\pi^3\,\delta_2-2\,i\,\pi\,\mathrm{HPL}\left[\{0,0\},\frac{1}{X}\right]\delta_2-i\,\pi\,\mathrm{HPL}\left[\{\mathrm{minus},0\},\frac{1}{X}\right]\delta_2+\pi^2\,\mathrm{HPL}\left[\{0\},\frac{1}{X}\right]\delta_2^2+\frac{1}{2}\pi^2\,\mathrm{HPL}\left[\{\mathrm{minus}\},\frac{1}{X}\right]\delta_2^2+\frac{1}{2}\,i\,\pi^3\,\delta_2^3-\frac{1}{16}\,i\,\delta_2\,\mathrm{Zeta}\left[3,\frac{1}{4}\right]+\frac{1}{16}\,i\,\delta_2\,\mathrm{Zeta}\left[3,\frac{3}{4}\right]$$

The transformations available are the same as for `HPLConvertToSimplerArgument`, with the same restrictions on the weight vector.

```
HPLArgTransform[HPL[{2, -1}, X], x → √x]
HPLArgTransform::WrongWeight :
 The argument transformation X → √X attempted is not defined for the weight vector {2, -1}
HPL[{2, -1}, X]
HPLArgTransform[HPL[{1, -1, 2}, X], x → 1 - x]
HPLArgTransform::WrongWeight :
 The argument transformation X → 1 - X attempted is not defined for the weight vector {1, -1, 2}
HPL[{1, -1, 2}, X]
```

The rule $r$ can be written using any symbol, which makes the code more intuitive. The symbol in the rule does not have to match the arguments of the HPLs.

```
HPLArgTransform[HPL[{2, 3}, -√x], t → -t]
HPL[{-2, -3}, √x]
HPLArgTransform[HPL[{2, 3}, 9 / 10], x → 1 - x]
```

$$\frac{1}{72}\pi^4\,\mathrm{HPL}\left[\{1\},\frac{1}{10}\right]-\frac{1}{6}\pi^2\,\mathrm{HPL}\left[\{1,2\},\frac{1}{10}\right]-\mathrm{HPL}\left[\{1,2,1,0\},\frac{1}{10}\right]-\frac{1}{3}\pi^2\,\mathrm{Zeta}[3]+\mathrm{HPL}\left[\{1,0\},\frac{1}{10}\right]\mathrm{Zeta}[3]+\frac{9\,\mathrm{Zeta}[5]}{2}$$

```
HPLArgTransform[HPL[{-2}, 1/(1 - y^2)], t → 1 / t]
```

$$\frac{\pi^2}{6}-\mathrm{HPL}\left[\{-2\},1-y^2\right]+\mathrm{HPL}\left[\{0,0\},1-y^2\right]$$

- `HPLReduceToMinimalSet` returns its argument with the HPLs projected to the minimal set, as described in Section 2.2.1.

```
HPLReduceToMinimalSet[HPL[{1, 2, 3}, x]]
HPL[{2}, x]^3 - 4 HPL[{3}, x] HPL[{2, 1}, x] - HPL[{2}, x] HPL[{2, 2}, x] +
 HPL[{1}, x] HPL[{2, 3}, x] + 2 HPL[{2, 1, 3}, x] - 2 HPL[{2, 3, 1}, x]
HPLReduceToMinimalSet[HPL[{minus, minus, 0}, x]]
```

$$\frac{1}{2}\left(\mathrm{HPL}[\{0\},x]\,\mathrm{HPL}[\{\mathrm{minus}\},x]^2-2\left(\mathrm{HPL}[\{\mathrm{minus}\},x]\,\mathrm{HPL}[\{0,\mathrm{minus}\},x]-\mathrm{HPL}[\{0,\mathrm{minus},\mathrm{minus}\},x]\right)\right)$$

- `HPLAnalyticContinuation[x_,HPLAnalyticContinuationRegion->region]` assumes that the arguments of the HPLs are real and returns its argument `x` with HPLs replaced by their analytic continuation, as described in Section 2.2.2. The arguments of the HPLs are taken to belong to the interval specified by the option `HPLAnalyticContinuationRegion`, for which `region` can be either

`minftom1` the interval $-\infty$ to $-1$

`m1to0` the interval $-1$ to $0$

`onetoinf` the interval $1$ to $\infty$.

The HPLs are replaced by their representation in terms of HPLs of argument in the interval $(0, 1)$. The choice of the side of the branch cut from which the argument is approached is set by the option

`HPLAnalyticContinuationSign`

which can take values $-1$, $1$ or any symbol.

```
HPLAnalyticContinuation[HPL[{0}, y],
 AnalyticContinuationRegion → m1to0, AnalyticContinuationSign → 1]
```

$i\pi + \mathrm{HPL}[\{0\}, -y]$

```
Simplify[HPLAnalyticContinuation[HPL[{1, -1}, y],
  AnalyticContinuationRegion → onetoinf, AnalyticContinuationSign → -1]]
```

$$-\frac{\pi^2}{4} - \mathrm{HPL}\left[\{0\}, \frac{1}{y}\right]^2 - \mathrm{HPL}\left[\{0\}, \frac{1}{y}\right] \mathrm{HPL}\left[\{1\}, \frac{1}{y}\right] + \mathrm{HPL}\left[\{-1\}, \frac{1}{y}\right] \left(\mathrm{HPL}\left[\{0\}, \frac{1}{y}\right] + \mathrm{HPL}\left[\{1\}, \frac{1}{y}\right]\right) + \mathrm{HPL}\left[\{2\}, \frac{1}{y}\right] - \mathrm{HPL}\left[\{-1, 0\}, \frac{1}{y}\right] - \mathrm{HPL}\left[\{-1, 1\}, \frac{1}{y}\right] + \mathrm{HPL}\left[\{0, 0\}, \frac{1}{y}\right] - i\pi\,\mathrm{Log}[2]$$

If the option `HPLAnalyticContinuationRegion` is omitted, and if the argument is numerical, `HPLAnalyticContinuation` will automatically use the appropriate setting. If the option `HPLAnalyticContinuationSign` is omitted, `HPLAnalyticContinuation` will use the value stored in the variable `$HPLAnalyticContinuationSign` which is set by default to 1[4].

```
HPLAnalyticContinuation[HPL[{1}, 3/2], AnalyticContinuationSign → -1]
```

$$-i\pi + \mathrm{HPL}\left[\{0\}, \frac{2}{3}\right] + \mathrm{HPL}\left[\{1\}, \frac{2}{3}\right]$$

```
Simplify[HPLAnalyticContinuation[HPL[{1, 0}, -5/2]]]
```

$$-\frac{\pi^2}{3} - \mathrm{HPL}\left[\{0\}, -\frac{2}{5}\right]^2 - \mathrm{HPL}\left[\{0\}, -\frac{2}{5}\right] \mathrm{HPL}\left[\{1\}, -\frac{2}{5}\right] + \mathrm{HPL}\left[\{2\}, -\frac{2}{5}\right] + \mathrm{HPL}\left[\{0, 0\}, -\frac{2}{5}\right]$$

It is to be noted that the `Mathematica` conventions for the analytic continuation are not always the same as that of the `HPL` package. This is illustrated by the following example

```
HPL[{1}, 1.9]
0.105361 + 3.14159 i
-Log[1 - 1.9]
0.105361 - 3.14159 i
```

Here `HPL` takes the argument of the HPL to have an infinitesimal positive

[4]This is the same convention as ref. [45], but opposite to that of ref. [47]

imaginary part, whereas Mathematica take the argument of the logarithm to have a positive imaginary part. Since the substitution of HPLs through more common functions has precedence over the analytic continuation, the option

`$HPLAutoConvertToKnownFunctions`

can interfere with the analytic continuation.

```
$HPLAutoConvertToKnownFunctions = True;
HPLAnalyticContinuation[HPL[{0}, t],
 AnalyticContinuationSign → δ, AnalyticContinuationRegion → m1to0]
Log[t]
$HPLAutoConvertToKnownFunctions = False;
HPLConvertToKnownFunctions[HPLAnalyticContinuation[HPL[{0}, t],
  AnalyticContinuationSign → δ, AnalyticContinuationRegion → m1to0]]
i π δ + Log[-t]
```

This example shows that with the option

`$HPLAutoConvertToKnownFunctions`

set to `True` we lose control over the sign of the imaginary part (as in the first case it will now depend on `Mathematica`'s conventions).

- `MZV[m]` is the Multiple Zeta Value (see Section 2.2.8) corresponding to the index vector $m$. Their value in terms of mathematical constants are tabulated[5] up to weight 8 and systematically replaced. For higher weights, the cases covered by Appendix 2.A are also replaced.

```
Table[MZV[{n}], {n, 2, 8}]
```

$$\left\{\frac{\pi^2}{6}, \mathrm{Zeta}[3], \frac{\pi^4}{90}, \mathrm{Zeta}[5], \frac{\pi^6}{945}, \mathrm{Zeta}[7], \frac{\pi^8}{9450}\right\}$$

```
MZV[{-2, -2}]
```

$$-\frac{\pi^4}{480}$$

```
MZV[{3, 1, 3, 1, 3, 1}]
```

$$\frac{\pi^{12}}{43589145600}$$

- `HPLI[m]` is the HPL of weight vector `m` evaluated at argument $i$. Their values in terms of mathematical constants are tabulated up to weight 8 and systematically replaced. For higher weights, the cases covered by Appendix 2.E are also replaced.

- The function `$HPLOptions` gives a list of the options of the package and their current values.

```
$HPLOptions
{$HPLAnalyticContinuationSign → 1, $HPLAutoConvertToKnownFunctions → False,
 $HPLAutoConvertToSimplerArgument → False, $HPLAutoLogExtract → False,
 $HPLAutoProductExpand → False, $HPLAutoReduceToMinimalSet → False}
```

[5]these tables are those of the FORM package `harmpol` [43].

- The variable `$HPLFunctions` contains a list of the functions provided by the package.

```
$HPLFunctions
{HPL, HPLAnalyticContinuation, HPLAtoM, HPLConvertToKnownFunctions,
 HPLConvertToSimplerArgument, HPLLogExtract, HPLMtoA,
 HPLProductExpand, HPLReduceToMinimalSet, MZV, HPLpm21m1, HPL1m12pm}
```

## 2.3.2 Functions modified

- We define the derivatives of HPLs as described in Section 2.2.

$$\{\partial_x \mathrm{HPL}[\{2,10,4\},x],\ \partial_x \mathrm{HPL}[\{-1,4,-6\},x],\ \partial_x \mathrm{HPL}[\{1,3,7\},x]\}$$

$$\left\{\frac{\mathrm{HPL}[\{1,10,4\},x]}{x},\ \frac{\mathrm{HPL}[\{4,-6\},x]}{1+x},\ \frac{\mathrm{HPL}[\{3,7\},x]}{1-x}\right\}$$

$$\{\partial_x \mathrm{HPL}[\{\mathrm{plus},\mathrm{minus},0\},x],\ \partial_x \mathrm{HPL}[\{\mathrm{minus},\mathrm{minus},\mathrm{plus}\},x]\}$$

$$\left\{\frac{2\,\mathrm{HPL}[\{\mathrm{minus},0\},x]}{1-x^2},\ \frac{2\,x\,\mathrm{HPL}[\{\mathrm{minus},\mathrm{plus}\},x]}{1-x^2}\right\}$$

The integration showing up in the recursive definition of the HPLs is also implemented.

$$\left\{\int_0^t \frac{\mathrm{HPL}[\{2,4\},x]}{1-x}\,dx,\ \int_0^t \frac{\mathrm{HPL}[\{2,4\},x]}{x}\,dx,\ \int_0^t \frac{\mathrm{HPL}[\{2,4\},x]}{1+x}\,dx\right\}$$

$$\{\mathrm{HPL}[\{1,2,4\},t],\ \mathrm{HPL}[\{3,4\},t],\ \mathrm{HPL}[\{-1,2,4\},t]\}$$

$$\left\{\int_0^t \frac{2\,x\,\mathrm{HPL}[\{0,\mathrm{minus}\},x]}{1-x^2}\,dx,\ \int_0^t \frac{2\,\mathrm{HPL}[\{\mathrm{plus},0,\mathrm{minus}\},x]}{1-x^2}\,dx\right\}$$

$$\{\mathrm{HPL}[\{\mathrm{minus},0,\mathrm{minus}\},t],\ \mathrm{HPL}[\{\mathrm{plus},\mathrm{plus},0,\mathrm{minus}\},t]\}$$

- The function `Series` is able to expand HPLs around $x = 0$ and $x = 1$.

$$\mathrm{Series}[\mathrm{HPL}[\{2,3,4,5\},x],\{x,0,7\}]$$

$$\frac{x^4}{6912}+\frac{193\,x^5}{1382400}+\frac{1026311\,x^6}{8957952000}+\frac{241822151\,x^7}{2633637888000}+O[x]^8$$

$$\mathrm{Series}[\mathrm{HPL}[\{1,2,3\},x],\{x,1,1\}]$$

$$\left(-\frac{143\,\pi^6}{45360}+\frac{1}{3}\pi^2\,\mathrm{Log}[1-x]\,\mathrm{Zeta}[3]+\mathrm{Zeta}[3]^2-\frac{9}{2}\mathrm{Log}[1-x]\,\mathrm{Zeta}[5]\right)+\left(-\frac{\pi^4}{72}+2\,\mathrm{Zeta}[3]-\mathrm{Log}[1-x]\,\mathrm{Zeta}[3]\right)(1-x)+O[1-x]^2$$

$$\mathrm{Series}[\mathrm{HPL}[\{\mathrm{plus},\mathrm{minus}\},x],\{x,0,17\}]$$

$$\frac{2\,x^3}{3}+\frac{3\,x^5}{5}+\frac{11\,x^7}{21}+\frac{25\,x^9}{54}+\frac{137\,x^{11}}{330}+\frac{49\,x^{13}}{130}+\frac{121\,x^{15}}{350}+\frac{761\,x^{17}}{2380}+O[x]^{18}$$

$$\mathrm{Series}[\mathrm{HPL}[\{\mathrm{plus},\mathrm{minus}\},x],\{x,1,2\}]$$

$$\left(\frac{\pi^2}{6}-\frac{3\,\mathrm{Log}[2]^2}{2}+\mathrm{Log}[2]\,\mathrm{Log}[1-x]+\frac{1}{2}\mathrm{Log}[1-x]^2\right)+\left(-1+\frac{\mathrm{Log}[2]}{2}+\frac{1}{2}\mathrm{Log}[1-x]\right)(1-x)+\left(-\frac{1}{4}+\frac{\mathrm{Log}[2]}{8}+\frac{1}{8}\mathrm{Log}[1-x]\right)(1-x)^2+O[1-x]^3$$

### 2.3.3 Working with options

The package HPL has some options to control its behavior. They set the preferred form in which expressions are displayed. The option can be overridden locally by the functions described above. The effects of the options are described in the following.

`$HPLAutoConvertToKnownFunctions`: If set to `True`, HPLs will be converted to more common functions (logs, polylogarithms, Nielsen polylogs) if possible, using the identities of Appendix 2.D. This might be counterproductive when the properties of the HPLs are more explicit in the HPL form than other representations.

```
$HPLAutoConvertToKnownFunctions = False;
HPL[{plus}, x]
HPL[{3, 1, 1}, t] + HPL[{-1, 1}, x]
HPL[{plus}, x]
HPL[{-1, 1}, x] + HPL[{3, 1, 1}, t]
$HPLAutoConvertToKnownFunctions = True;
HPL[{minus}, x]
HPL[{3, 1, 1}, t] + HPL[{-1, 1}, x]
```

$-\mathrm{Log}[1-x^2]$

$-\frac{\pi^2}{12}+\frac{\mathrm{Log}[2]^2}{2}-\mathrm{Log}[2]\,\mathrm{Log}[1+x]+\mathrm{PolyLog}\left[2,\frac{1+x}{2}\right]+\mathrm{PolyLog}[2,3,t]$

Furthermore, if this options is set to `True` while using the analytic continuation described above, the result may be wrong, as `Mathematica` does not have different conventions for the analytic continuation. Default is `False`.

`$HPLAutoProductExpand`: If `True` the products of HPLs are automatically converted into a sum of HPL of weight equal to the sum of the weights of the two factors, as described in section 2.2.1. Default is `False`.

```
$HPLAutoProductExpand = False;
HPL[{plus}, t] HPL[{minus, 0}, t]
HPL[{plus}, t] HPL[{minus, 0}, t]
$HPLAutoProductExpand = True;
HPL[{plus}, t] HPL[{minus, 0}, t]
HPL[{minus, 0, plus}, t] + HPL[{minus, plus, 0}, t] + HPL[{plus, minus, 0}, t]
```

Setting the option `$HPLAutoProductExpand True` affects only explicit products and does not act on factorized products like the function `HPLProductExpand`.

```
HPL[{-1, 1}, t] (HPL[{1}, t] + t)
(t + HPL[{1}, t]) HPL[{-1, 1}, t]
Expand[%]
t HPL[{-1, 1}, t] + 2 HPL[{-1, 1, 1}, t] + HPL[{1, -1, 1}, t]
```

`$HPLAutoLogExtract`: If `True` the logarithmic divergences $\log(1-x)$ and $\log(x)$ are automatically extracted from the HPLs following the procedure described in Section 2.2.2. The default setting is `False`.

```
$HPLAutoLogExtract = False;
HPL[{plus, 0}, t]
HPL[{1, -2}, t]

HPL[{plus, 0}, t]

HPL[{1, -2}, t]

$HPLAutoLogExtract = True;
HPL[{plus, 0}, t]
HPL[{1, -2}, t]

HPL[{0}, t] HPL[{plus}, t] - HPL[{0, plus}, t]

HPL[{-2}, t] HPL[{1}, t] - HPL[{-2, 1}, t] - HPL[{2, -1}, t]
```

The extraction of the divergent behavior only makes sense, if one does not re-expand the products automatically with the option `$HPLAutoProductExpand` set to `True`. If the latter option is set to `True`, the option `$HPLAutoLogExtract` will have no effect.

```
$HPLAutoLogExtract = True;

$HPLAutoProductExpand = True;

HPL[{1, -2}, t]

HPL[{1, -2}, t]

$HPLAutoProductExpand = False;

HPL[{1, -2}, t]

HPL[{-2}, t] HPL[{1}, t] - HPL[{-2, 1}, t] - HPL[{2, -1}, t]
```

On the other hand, if the option `$HPLAutoConvertToKnownFunctions` is set to `True`, the out factorized HPLs of weight one will be replaced by logs before being re-expanded, as shown by the following example.

```
$HPLAutoLogExtract = True;

$HPLAutoConvertToKnownFunctions = True;
HPL[{1, 4, 4}, t]
HPL[{minus, plus, 0}, t]
-HPL[{2, 3, 4}, t] - HPL[{3, 2, 4}, t] - 2 HPL[{4, 1, 4}, t] - HPL[{4, 2, 3}, t] -
 HPL[{4, 3, 2}, t] - 2 HPL[{4, 4, 1}, t] - HPL[{4, 4}, t] Log[1 - t]

-HPL[{0, minus, plus}, t] - HPL[{minus, 0, plus}, t] + HPL[{minus, plus}, t] Log[t]
```

`$HPLAutoReduceToMinimalSet`: If set to `True`, the HPLs will be automatically reduced to a minimal basis (up to weight 8). This only makes sense if one does not expand the obtained products again, or if the factors of smaller weight can be replaced by their expression in terms of known functions. Therefore, for the reduction to be performed, one has to have the option

`$HPLAutoProductExpand` equal to `False` or

`$HPLAutoConvertToKnownFunctions` equal to `True`.

If this is not fulfilled, the option will have no effect. It defaults to `False`.

```
$HPLAutoReduceToMinimalSet = False;
HPL[{plus, 0, minus, plus}, x]
HPL[{1, 2, 1}, x]

HPL[{plus, 0, minus, plus}, x]

HPL[{1, 2, 1}, x]

$HPLAutoReduceToMinimalSet = True;
HPL[{plus, 0, minus}, x]
HPL[{1, 2, 1}, x]

HPL[{plus}, x] HPL[{0, minus}, x] - HPL[{0, minus, plus}, x] - HPL[{0, plus, minus}, x]

HPL[{1}, x] HPL[{2, 1}, x] - 3 HPL[{2, 1, 1}, x]
```

`$HPLAutoConvertToSimplerArgument`: If set to `True`, HPLs of arguments $-x$, $x^2$, $1-x$, $1/x$, $x/(x-1)$ and $(1-x)/(1+x)$ will be automatically replaced by their representation in term of HPLs of argument $x$ along the lines of appendix 2.2.6. Its default is `False`.

```
$HPLAutoConvertToSimplerArgument = False;
HPL[{1, 2}, 1 - x]
HPL[{plus, 0, minus}, 1 / x]
```

$$-\text{HPL}[\{0\},x]\left(\frac{\pi^2}{6}+\text{HPL}[\{1,0\},x]\right)-2\,(-\text{HPL}[\{1,0,0\},x]+\text{Zeta}[3])$$

$$-\frac{i\,\pi^3}{24}+\frac{1}{6}\pi^2\,\text{HPL}[\{\text{plus}\},x]-i\,\pi\,\text{HPL}[\{\text{plus},0\},x]-2\,\text{HPL}[\{\text{plus},0,0\},x]-\text{HPL}[\{\text{plus},0,\text{minus}\},x]-\frac{1}{16}\,i\,\text{Zeta}\left[3,\frac{1}{4}\right]+\frac{1}{16}\,i\,\text{Zeta}\left[3,\frac{3}{4}\right]$$

```
$HPLAutoConvertToSimplerArgument = True;
HPL[{1, 2}, 1 - x]
```

$$-\text{HPL}[\{0\},x]\left(\frac{\pi^2}{6}+\text{HPL}[\{1,0\},x]\right)-2\,(-\text{HPL}[\{1,0,0\},x]+\text{Zeta}[3])$$

`$HPLAnalyticContinuationSign`: If set to 1 the analytic continuation of the HPLs is taken assuming a positive infinitesimal imaginary part for arguments, if set to $-1$ a negative one is assumed. `$HPLAnalyticContinuationSign` is only the default setting and can be overridden by specifying the option `AnalyticContinuationSign` in the function `HPLAnalyticContinuation`, as described above. `$HPLAnalyticContinuationSign` can be a symbol. The default setting is $+1$.

```
$HPLAnalyticContinuationSign

1

HPL[{0}, -1]

i π

$HPLAnalyticContinuationSign = -δ;
HPL[{0}, -1]

-i π δ
```

### 2.3.4 Numerical evaluation

The package HPL 2 provides an arbitrary-precision numerical evaluation in the whole complex plane.

#### Real argument

HPLs of real arguments with finite precision are automatically evaluated to the precision of the argument.

```
HPL[{2, 1, 4, 5}, 0.5]
HPL[{0, plus, minus, 0, minus}, 0.5]
0.000174907
0.000809316
HPL[{2, 1, 4, 5}, 1/2.`30.]
HPL[{0, plus, minus, 0, minus}, 1/2.`30.]
0.000174907282457760677740168010076
0.000809316225590848646790730451150
```

For arguments with infinite precision, numerical evaluation is only undertaken if explicitly requested.

```
HPL[{2, 1, 4, 5}, 1/2]
HPL[{plus, minus, 0, minus}, 1/2]
HPL[{2, 1, 4, 5}, 1/2]
HPL[{plus, minus, 0, minus}, 1/2]
N[HPL[{2, 1, 4, 5}, 1/2], 50]
N[HPL[{0, plus, minus, 0, minus}, 1/2], 50]
0.00017490728245776067774016801007622686190198808601431
0.00080931622559084864679073045114617672882050519276148
```

For the numerical values of the MZV, we implemented the procedure described in refs. [47, 48].

```
N[MZV[{4, 3}]]
0.0851598
N[MZV[{2, 5, 4, 3}], 40]
0.0000971639689998491980155438399782847850253 2
```

For real arguments outside the interval $[0, 1]$, one can specify the sign of the infinitesimal imaginary part to be used for the analytic continuation by appending the option AnalyticContinuationSign as for the function HPLAnalyticContinuation.

```
HPL[{2, 1, 0}, 1.4, AnalyticContinuationSign → 1]
HPL[{minus, plus, 0}, 1.4, AnalyticContinuationSign → 1]
-1.99573 - 1.73879 i
1.08233 - 7.75157 i
HPL[{2, 1, 0}, 1.4, AnalyticContinuationSign → -1]
HPL[{minus, plus, 0}, 1.4, AnalyticContinuationSign → -1]
-1.99573 + 1.73879 i
1.08233 + 7.75157 i
```

### Complex argument

For the sake of the numerical evaluation for complex arguments, we divide the complex plane into five different regions as pictured by figure 2.3.4.

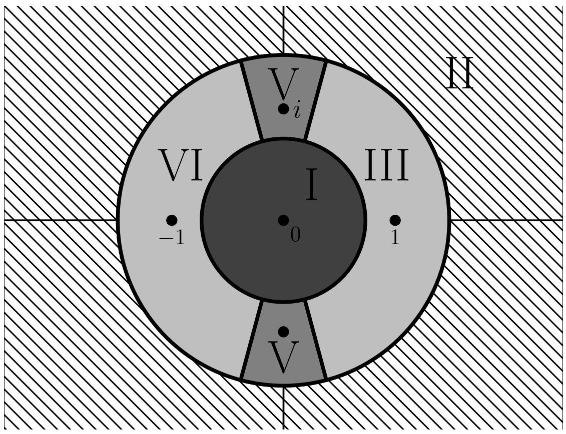



Figure 2.1: Complex plane division for the numerical evaluation

**region I:** $|z| < 0.9$
: the series expansion is used

**region II:** $|z| > 1.5$
: First the argument is brought into region I using the argument transformation $z \to 1/z$ described in Section 2.2.6, then the HPLs are evaluated using series expansions.

**region III:** $0.9 < |z| < 1.5$ **and** $|\arg(z)| < 5\pi/12$
: First the argument is brought into region I using the argument transformation $z \to (1-z)/(1+z)$ described in Section 2.2.6, then the HPLs are evaluated using series expansions.

**region IV:** $0.9 < |z| < 1.5$ **and** $|\arg(z)| > 7\pi/12$
: First the argument is brought into region I using the argument transformations $z \to -z$ and $z \to (1-z)/(1+z)$ described in Section 2.2.6, then the HPLs are evaluated using series expansions.

**region V:** $0.9 < |z| < 1.5$ **and** $5\pi/12 < |\arg(z)| < 7\pi/12$
The evaluation is done using the Hölder convolution described in ref. [48].

The transformations mentioned above are performed using the "complex" argument transformation for the $+-$ weights and the "real" transformations for integer weights. The evaluation for the $+-$ weights in region V is done by first converting to the integer weights and then using the Hölder convolution.

HPLs with numerical complex arguments with finite precision are evaluated automatically.

```
HPL[{1, -2, 3}, 0.5 ⅈ + 0.7]
HPL[{plus, minus, 0}, 0.5 ⅈ + 0.7]

-0.05413 + 0.0438294 ⅈ

0.1566 - 0.508478 ⅈ
HPL[{1, -2, 3}, 1.5 ⅈ + 1.7]
HPL[{plus, minus, 0}, 1.5 ⅈ + 1.7]

-0.503607 - 0.252553 ⅈ

1.70143 - 1.07863 ⅈ
```

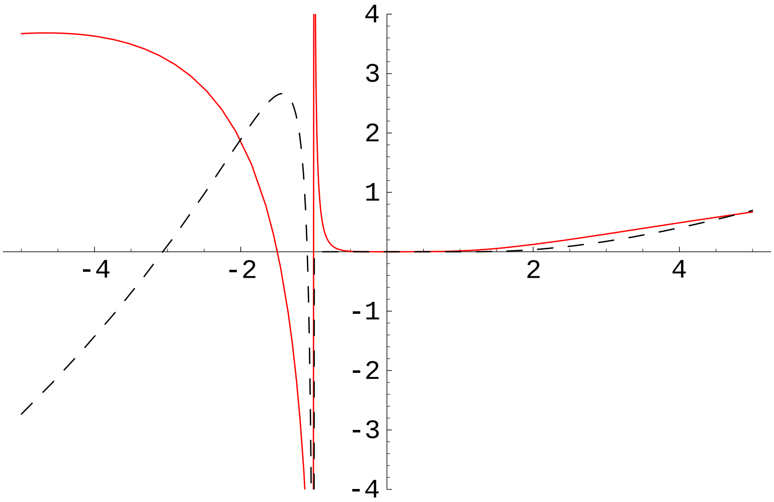
HPLs with complex argument with infinite precision are only evaluated if explicitly requested.

```
N[HPL[{3, -2, 1}, 13 + 7 ⅈ], 50]
-2.6346279281243037714092494101947734783554557274122 -
 2.7289184907880926000947141638056212522510887136916 ⅈ

N[HPL[{0, plus, minus, plus}, 13 + 7 ⅈ], 50]
6.8060017197430759251833294345157620921643906833439 -
 6.4915066233930765780643429173450624350255531622085 ⅈ
```

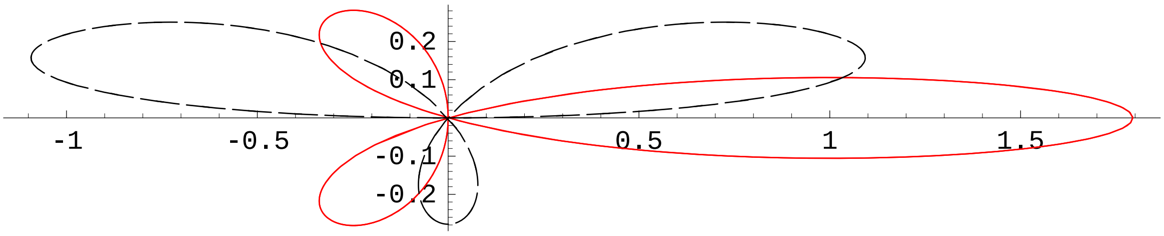
Thanks the possibility of evaluating the HPLs numerically, `Plot` is able to represent HPLs graphically on the real axis

```
Plot[{Re[HPL[{-1, -1, -1, 1}, t]], Im[HPL[{-1, -1, -1, 1}, t]]},
 {t, -5, 5}, PlotStyle → {Hue[1], Dashing[{0.02, 0.02}]}, PlotRange → {-4, 4}]
```

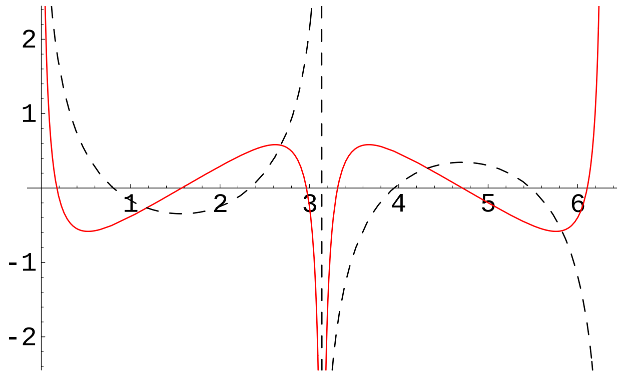



and in the complex plane, here are two examples of HPLs plotted on the interval $[-5, 5]$ and in the unit circle

```
PolarPlot[{Re[HPL[{plus, minus}, 9 / 10 ⅇ^(ⅈ θ)]], Im[HPL[{plus, minus}, 9 / 10 ⅇ^(ⅈ θ)]]},
 {θ, 0, 2 π}, PlotStyle → {Hue[1], Dashing[{0.02, 0.02}]}]
```




```
Plot[{Re[HPL[{plus, minus}, ⅇ^(ⅈ θ)]], Im[HPL[{plus, minus}, ⅇ^(ⅈ θ)]]},
 {θ, 0, 2 π}, PlotStyle → {Hue[1], Dashing[{0.02, 0.02}]}]
```




We checked numerical agreement with ref. [45] at double precision accuracy. The values of the MZV have been checked against those of the `EZface` application [51] and the GiNaC implementation [47]. Concerning speed, our implementation cannot be expected to compete with the GiNaC implementation.

## 2.4 Conclusion and outlook

In this chapter we presented the harmonic polylogarithm and extended them to the complex plane. We have defined new weights that are more suited for complex argument, as will be shown in the next chapter. We also presented the Mathematica implementation `HPL` that allows the use of harmonic polylogarithms in the framework of Mathematica.

The first version of the package `HPL` for real arguments has been used for various applications like corrections to Higgs production and decay [52, 53], computation of master integrals [37], heavy quark forward-backward asymmetry [54, 55] and form factors [56], corrections to Bhabha scattering [57], lepton $g-2$ [58], large-$x$ limit of parton evolution [59] and various loop calculations [60–62].

## 2.A Multiple zeta values and colored MZV

We list here some of the identities for MZVs found in refs. [48, 49]. These identities are used automatically,

$$\zeta(2,1) = \zeta(3)\ , \tag{2.38}$$

$$\zeta(4,2) = \zeta^2(3) - \frac{4\pi^6}{2835}\ , \tag{2.39}$$

$$2\zeta(m,1) = m\zeta(m+1) - \sum_{k=1}^{m-2}\zeta(m-k)\zeta(k+1),\quad 2\le m\in\mathbb{Z}\ , \tag{2.40}$$

$$\zeta(2,{}^n1) = \zeta(n+2)\ , \tag{2.41}$$

$$\begin{aligned}\zeta(3,{}^n1) &= \zeta(n+2,1)\\ &= \frac{n+2}{2}\zeta(n+3) - \frac{1}{2}\sum_{k=1}^{n}\zeta(k+1)\zeta(n+2-k)\ ,\end{aligned} \tag{2.42}$$

$$\zeta({}^n2) = \frac{2(2\pi)^{2n}}{(2n+1)!}\left(\frac{1}{2}\right)^{2n+1}\ , \tag{2.43}$$

$$\zeta({}^n4) = \frac{4(2\pi)^{4n}}{(4n+2)!}\left(\frac{1}{2}\right)^{2n+1}\ , \tag{2.44}$$

$$\zeta({}^n6) = \frac{6(2\pi)^{6n}}{(6n+3)!}\ , \tag{2.45}$$

$$\zeta({}^n8) = \frac{8(2\pi)^{8n}}{(8n+4)!}\left\{\left(1+\frac{1}{\sqrt{2}}\right)^{4n+2} + \left(1-\frac{1}{\sqrt{2}}\right)^{4n+2}\right\}\ , \tag{2.46}$$

$$\zeta({}^n\{3,1\}) = 4^{-n}\zeta({}^n4) = \frac{2\pi^{4n}}{(4n+2)!}\ , \tag{2.47}$$

$$\begin{aligned}\zeta(2,{}^n\{1,3\}) &= 4^{-n}\sum_{k=0}^{n}(-1)^k\zeta(\{4\}^n)\big\{(4k+1)\zeta(4k+2)\\ &\qquad -4\sum_{j=1}^{k}\zeta(4j-1)\zeta(4k-4j+3)\big\}\ ,\end{aligned} \tag{2.48}$$

where the sum in the last equation is over all non negative integers satisfying $\sum_{k\geq 0} kj_k = n$.

The identities with negative weights are the following,

$$\zeta({}^n(-2)) = \frac{\pi^{2n}}{(2n+1)!}\frac{(-1)^{n(n+1)/2}}{2^n}, \tag{2.49}$$

$$\zeta({}^n(-4)) = \frac{\pi^{4n}}{(4n+2)!}\frac{(-1)^{n(n+1)/2}}{2^n}\left(\left(1+\sqrt{2}\right)^{2n+1}+\left(1-\sqrt{2}\right)^{2n+1}\right), \tag{2.50}$$

$$\begin{aligned}\zeta({}^n(-6)) &= \frac{\pi^{6n}}{(6n+3)!}\frac{3}{2}\Big(1+2^{3n+1}(-1)^{n(n+1)/2} \\ &\quad \times\left\{\left(\frac{1+\sqrt{3}}{2}\right)^{6n+3}+\left(\frac{1-\sqrt{3}}{2}\right)^{6n+3}-1\right\}, \end{aligned}\tag{2.51}$$

$$\zeta({}^n(-1)) = (-1)^n\sum\prod_{k\geq 1}\frac{1}{j_k!}\left(\frac{-\mathrm{Li}_k((-1)^k)}{k}\right)^{j_k}, \tag{2.52}$$

$$\begin{aligned}\zeta(-1,{}^n1) &= (-1)^{n+1}\frac{(\log 2)^n}{n!}, \\ \zeta(-1,-1,{}^n1) &= -\mathrm{Li}_{n+2}(1/2). \end{aligned}\tag{2.53}$$

## 2.B Minimal set

MZVs can be expressed as linear combinations of mathematical constants such as $\pi$, $\zeta(n)$ or $\mathrm{Li}_n(1/2)$ and, for high weight, a minimal set of other constants. In the tables we translated [2], the following choice of constants in the minimal set has been used,

$$\begin{aligned} s_6 &= S(\{-5,-1\},\infty) = \sum_{i_1=1}^{\infty}\frac{(-1)^{i_1}}{i_1^5}\sum_{i_2=1}^{i_1}\frac{(-1)^{i_2}}{i_2} \\ &= \zeta(-5,-1)+\zeta(6) \simeq 0.98744142640329971377, \end{aligned}\tag{2.54}$$

$$\begin{aligned} s_{7a} &= S(\{-5,1,1\},\infty) = \sum_{i_1=1}^{\infty}\frac{(-1)^{i_1}}{i_1^5}\sum_{i_2=1}^{i_1}\frac{1}{i_2}\sum_{i_3=1}^{i_2}\frac{1}{i_3} \\ &= \zeta(-5,1,1)+\zeta(-6,1)+\zeta(-5,2)+\zeta(-7) \\ &\simeq -0.95296007575629860341, \end{aligned}\tag{2.55}$$

$$\begin{aligned} s_{7b} &= S(\{5,-1,-1\},\infty) = \sum_{i_1=1}^{\infty}\frac{1}{i_1^5}\sum_{i_2=1}^{i_1}\frac{(-1)^{i_2}}{i_2}\sum_{i_3=1}^{i_2}\frac{(-1)^{i_3}}{i_3} \\ &= \zeta(7)+\zeta(5,2)+\zeta(-6,-1)+\zeta(5,-1,-1) \\ &\simeq 1.02912126296432453422, \end{aligned}\tag{2.56}$$

$$
\begin{aligned}
s_{8a} &= S(\{5,3\},\infty) = \sum_{i_1=1}^{\infty} \frac{1}{i_1^5} \sum_{i_2=1}^{i_1} \frac{1}{i_2^3} \\
&= \zeta(8) + \zeta(5,3) \simeq 1.0417850291827918834\,, \\
s_{8b} &= S(\{-7,-1\},\infty) = \sum_{i_1=1}^{\infty} \frac{(-1)^{i_1}}{i_1^7} \sum_{i_2=1}^{i_1} \frac{(-1)^{i_2}}{i_2} \\
&= \zeta(8) + \zeta(-7,-1) \simeq 0.99644774839783766600\,, \qquad (2.57) \\
s_{8c} &= S(\{-5,-1,-1,-1\},\infty) \\
&= \sum_{i_1=1}^{\infty} \frac{(-1)^{i_1}}{i_1^5} \sum_{i_2=1}^{i_1} \frac{(-1)^{i_2}}{i_2} \sum_{i_3=1}^{i_2} \frac{(-1)^{i_3}}{i_3} \sum_{i_3=1}^{i_3} \frac{(-1)^{i_4}}{i_4} \\
&= \zeta(8) + \zeta(-7,-1) + \zeta(-5,-3) + \zeta(6,2) + \zeta(-5,-1,2) \\
&\quad +\zeta(-5,2,-1) + \zeta(6,-1,-1) + \zeta(-5,-1,-1,-1) \qquad (2.58) \\
&\simeq 0.98396667382173367094\,, \\
s_{8d} &= S(\{-5,-1,1,1\},\infty) = \sum_{i_1=1}^{\infty} \frac{(-1)^{i_1}}{i_1^5} \sum_{i_2=1}^{i_1} \frac{(-1)^{i_2}}{i_2} \sum_{i_3=1}^{i_2} \frac{1}{i_3} \sum_{i_3=1}^{i_3} \frac{i}{i_4} \\
&= \zeta(8) + \zeta(-5,-3) + \zeta(6,2) + \zeta(7,1) + \zeta(-5,-2,1) + \zeta(-5,-1,2) \\
&\quad +\zeta(6,1,1) + \zeta(-5,-1,1,1) \simeq 0.99996261346268344768\,. \qquad (2.59)
\end{aligned}
$$

## 2.C Conversion of HPL at unity to MZV

In this appendix we prove the formulae presented in 2.2.8. We first prove

$$
\begin{aligned}
H(-m;1) &= -\zeta(-m) = \sum_{i=1}^{\infty} \frac{(-1)^{i+1}}{i^m} \\
&= -\sum_{i=1}^{\infty} \frac{1}{(2i)^m} - \sum_{i=1}^{\infty} \frac{-1}{(2i-1)^m} \\
&= -2^{-m}\zeta(m) + (\sum_{i=1}^{\infty} \frac{1}{i^m} - \sum_{i=1}^{\infty} \frac{1}{(2i)^m} \\
&= -2^{-m}\zeta(m) + \big(\zeta(m) - 2^{-m}\zeta(m)\big) \\
&= (1-2^{1-m})\zeta(m)\,. \qquad (2.60)
\end{aligned}
$$

For the proof of the formula for higher depth we start with the definition (2.15) of the coefficients of the series expansion of the HPL and first prove that

$$
(-1)^{i+1} Z_i(m_{1,\dots,k}) = (-1)^{k+1} Z_i(-m_{1,\dots,k}). \qquad (2.61)
$$

This holds for depth 1,

$$(-1)^{i+1} Z_i(m_1) = (-1)^{i+1} \frac{\mathrm{sgn}(m_1)^{i+1}}{i^{|m|}}$$
$$= \begin{cases} (-1)^{i+1} \dfrac{1}{i^{m_1}} = Z_i(-m_1), & m_1 > 0 \\ \\ (-1)^{i+1} \dfrac{(-1)^{i+1}}{i^{|m_1|}} = \dfrac{1}{i^{-m_1}} = Z_i(-m_1), & m_1 < 0\ . \end{cases} \tag{2.62}$$

For $m_{1,\ldots,k}$ with $m_1 > 0$ we get

$$\begin{aligned} &(-1)^{i+1} Z_1(m_{1,\ldots,k}) = \\ &= (-1)^{i+1} \frac{1}{i^{m_1}} \sum_{i_2=1}^{i-1} Z_{i_2}(m_{2,\ldots,k}) \\ &= -\frac{(-1)^i}{i^{m_1}} \sum_{i_2=1}^{i-1} (-1)^{i_2+1} (-1)^k Z_{i_2}(-m_{2,\ldots,k}) \\ &= (-1)^{k+1} Z_i(-m_{1,\ldots,k})\ , \end{aligned} \tag{2.63}$$

and for $m_1 < 0$,

$$\begin{aligned} (-1)^{i+1} Z_1(m_{1,\ldots,k}) = &= (-1)^{i+1} \frac{(-1)^{i+1}}{i^{|m_1|}} \sum_{i_2=1}^{i-1} (-1)^{i_2+1} Z_{i_2}(m_{2,\ldots,k}) \\ &= \frac{(1}{i^{|m_1|}} \sum_{i_2=1}^{i-1} (-1)^k Z_{i_2}(-m_{2,\ldots,k}) \\ &= (-1)^{k+1} Z_i(-m_{1,\ldots,k}). \end{aligned} \tag{2.64}$$

The next step is to prove for $k > 1$ that

$$Z_i(m_{1,\ldots,k}) = \\ N(m_{1,\ldots,k}) \frac{\mathrm{sgn}(m_1)^i}{i^{|m_1|}} \sum_{i_2=1}^{i-1} \cdots \sum_{i_k}^{i_{k-1}-1} \frac{\mathrm{sgn}(m_1 m_2)^{i_2}}{i_2^{|m_2|}} \cdots \frac{\mathrm{sgn}(m_{k-1} m_k)^{i_k}}{i_k^{|m_k|}}\ , \tag{2.65}$$

where $N(m_{1,\ldots,k})$ is given by $(-1)^{\#n}$ with $\#n$ the number of negative indices in the index vector $m$.

The proof is again through induction in the depth. We first test the claim for depth 2. For $m_1$ positive

$$
\begin{aligned}
Z_i(m_1, m_2) &= \frac{1}{i^{m_1}} \sum_{i_2=1}^{i-1} Z_{i_2}(m_2) = \frac{1}{i^{m_1}} \sum_{i_2=1}^{i-1} \frac{\mathrm{sgn}(m_2)^{i_2+1}}{i^{|m_2|}} \\
&= \begin{cases} \dfrac{1}{i^{m_1}} \displaystyle\sum_{i_2=1}^{i-1} \frac{1}{i^{m_2}} & m_2 > 0 \\[2ex] \dfrac{1}{i^{m_1}} \displaystyle\sum_{i_2=1}^{i-1} \frac{(-1)^{i_2+1}}{i^{|m_2|}} = -\frac{1}{i^{m_1}} \sum_{i_2=1}^{i-1} \frac{(-1)^{i_2}}{i^{|m_2|}} & m_2 < 0 \ , \end{cases}
\end{aligned} \tag{2.66}
$$

which is the expected result. For $m_1$ negative one has

$$
\begin{aligned}
Z_i(m_1, m_2) &= \frac{(-1)^i}{i^{|m_1|}} \sum_{i_2=1}^{i-1} Z_{i_2}(m_2) = \frac{(-1)^i}{i^{|m_1|}} \sum_{i_2=1}^{i-1} \frac{\mathrm{sgn}(m_2)^{i_2+1}}{i^{|m_2|}} \\
&= \begin{cases} \dfrac{(-1)^i}{i^{|m_1|}} \displaystyle\sum_{i_2=1}^{i-1} \frac{1}{i^{m_2}} & m_2 < 0 \\[2ex] \dfrac{(-1)^i}{i^{|m_1|}} \displaystyle\sum_{i_2=1}^{i-1} \frac{(-1)^{i_2+1}}{i^{|m_2|}} = -\frac{(-1)^i}{i^{|m_1|}} \sum_{i_2=1}^{i-1} \frac{(-1)^{i_2}}{i^{|m_2|}} & m_2 > 0 \ . \end{cases}
\end{aligned} \tag{2.67}
$$

We turn now to the general case $k > 2$. For $m_1$ positive, one has

$$
\begin{aligned}
Z_i(m_{1,\dots,k}) &= \frac{1}{i^{m_1}} \sum_{i_2=1}^{i-1} Z_{i_2}(m_{2,\dots,k}) \\
&= \frac{1}{i^{m_1}} N(m_{2,\dots,k}) \sum_{i_2=1}^{i-1} \cdots \sum_{i_k}^{i_{k-1}-1} \frac{\mathrm{sgn}(m_2)^{i_2}}{i_2^{|m_2|}} \frac{\mathrm{sgn}(m_2 m_3)^{i_3}}{i_3^{|m_3|}} \cdots \frac{\mathrm{sgn}(m_{k-1} m_k)^{i_k}}{i_k^{|m_k|}} \\
&= N(m_{1,\dots,k}) \frac{1}{i^{m_1}} \sum_{i_2=1}^{i-1} \cdots \sum_{i_k}^{i_{k-1}-1} \frac{\mathrm{sgn}(m_1 m_2)^{i_2}}{i_2^{|m_2|}} \cdots \frac{\mathrm{sgn}(m_{k-1} m_k)^{i_k}}{i_k^{|m_k|}},
\end{aligned} \tag{2.68}
$$

and for $m_1 < 0$

$$
\begin{aligned}
Z_i(m_{1,\ldots,k}) &= \frac{(-1)^i}{i^{|m_1|}} \sum_{i_2=1}^{i-1} (-1)^{i_2+1} Z_{i_2}(m_{2,\ldots,k}) \\
&= \frac{\mathrm{sgn}(m_1)^i}{i^{|m_1|}} \sum_{i_2=1}^{i-1} (-1)^k Z_{i_2}(-m_{2,\ldots,k}) \\
&= N(m_{2,\ldots,k})(-1)^k \frac{\mathrm{sgn}(m_1)^i}{i^{|m_1|}} \sum_{i_2=1}^{i-1} \cdots \sum_{i_k}^{i_{k-1}-1} \\
&\qquad \frac{-\mathrm{sgn}(m_2)^{i_2}}{i_2^{|m_2|}} \frac{\mathrm{sgn}((-m_2)(-m_3))^{i_2}}{i_2^{|m_2|}} \cdots \frac{\mathrm{sgn}((-m_{k-1})(-m_k))^{i_k}}{i_k^{|m_k|}} \\
&= N(m_{1,\ldots,k}) \frac{\mathrm{sgn}(m_1)^i}{i^{|m_1|}} \sum_{i_2=1}^{i-1} \cdots \sum_{i_k}^{i_{k-1}-1} \frac{\mathrm{sgn}(m_1 m_2)^{i_2}}{i_2^{|m_2|}} \cdots \frac{\mathrm{sgn}(m_{k-1} m_k)^{i_k}}{i_k^{|m_k|}} \,, \qquad (2.69)
\end{aligned}
$$

since

$$
\begin{aligned}
(-1)^k N(-m_{2,\ldots,k}) &= (-1)^{-k} (-1)^{k-1-\#n(m_{2,\ldots,k})} \\
&= (-1)^{-\#n(m_{2,\ldots,k}-1)} = (-1)^{\#n(m_{1,\ldots,k})} \,. \qquad (2.70)
\end{aligned}
$$

The connection between an HPL and the corresponding MZV is easy to figure out from the definition (2.34) of the MZV. One obtains the result (2.33)

$$
H(\{m_{1,\ldots,k}\}, 1) = N(m_{1,\ldots,k}) \zeta(\tilde{m}_{1,\ldots,k}). \qquad (2.71)
$$

## 2.D Table of representation through more common functions

In these tables, we collect identities relating HPLs to more common functions that can be found in refs. [32, 63]. These identities are used by the function `HPLConvertToKnownFunctions` (see Section 2.3.1) and applied systematically when the option `$HPLAutoConvertToKnownFunctions` is set to `True`, see Section 2.3.3.

### 2.D.1 Weight 2

$$
\begin{aligned}
H(\{1,1\};x) &= \frac{1}{2}\log(1-x)^2 \ , && (2.72)\\
H(\{1,-1\};x) &= \mathrm{Li}_2((1-x)/2) - \log(2)\log(1-x) - \mathrm{Li}_2\left(\frac{1}{2}\right) \ , && (2.73)\\
H(\{-1,1\};x) &= \mathrm{Li}_2((1+x)/2) - \log(2)\log(1+x) - \mathrm{Li}_2\left(\frac{1}{2}\right) \ , && (2.74)\\
H(\{-1,0\};x) &= \log(1+x)\log(x) + \mathrm{Li}_2(-x) \ , && (2.75)\\
H(\{-2\};x) &= -\mathrm{Li}_2(-x) \ . && (2.76)
\end{aligned}
$$

### 2.D.2 Weight 3

$$
\begin{aligned}
H(\{1,2\};x) &= -2S_{1,2}(x) - \log(1-x)\,\mathrm{Li}_2(x) \ , && (2.77)\\
H(\{1,1,1\};x) &= -\frac{1}{6}\log(1-x)^3 \ , && (2.78)\\
H(\{2,1\};x) &= S_{1,2}(x) \ , && (2.79)\\
H(\{2,-1\};x) &= \mathrm{Li}_3(\frac{2x}{1+x}) - \mathrm{Li}_3\left(\frac{x}{1+x}\right) - \mathrm{Li}_3\left(\frac{1+x}{2}\right)\\
&\quad -\mathrm{Li}_3(x) + \log(1+x)\mathrm{Li}_2(\frac{1}{2}) + \log(1+x)\mathrm{Li}_2(x)\\
&\quad +\frac{1}{2}\log(2)\log(1+x)^2 + \mathrm{Li}_3\left(\frac{1}{2}\right) \ , && (2.80)\\
H(\{-2,1\};x) &= -S_{1,2}(x) + \mathrm{Li}_3\left(\frac{-2x}{1-x}\right) - \mathrm{Li}_3\left(\frac{1-x}{2}\right) - \mathrm{Li}_3(-x)\\
&\quad +\mathrm{Li}_3\left(\frac{1}{2}\right) + \mathrm{Li}_3(x) + \log(1-x)\mathrm{Li}_2(-x)\\
&\quad +\log(1-x)\mathrm{Li}_2\left(\frac{1}{2}\right) - \log(1-x)\mathrm{Li}_2(x)\\
&\quad +\frac{1}{2}\log(2)\log(1-x)^2 - 1/6\log(1-x)^3 \ , && (2.81)\\
H(\{-2,-1\};x) &= S_{1,2}(-x) \ , && (2.82)\\
H(\{1,-1,-1\};x) &= -\frac{1}{2}\log\left(\frac{1-x}{2}\right)\log(1+x)^2 - \mathrm{Li}_3\left(\frac{1}{2}\right)\\
&\quad -\log(1+x)\mathrm{Li}_2\left(\frac{1+x}{2}\right) + \mathrm{Li}_3\left(\frac{1+x}{2}\right) \ . && (2.83)
\end{aligned}
$$

$$
\begin{aligned}
H(\{-1,1,1\};x) &= \frac{1}{2}\log\left(\frac{1+x}{2}\right)\log(1-x)^2+\mathrm{Li}_3\left(\frac{1}{2}\right) \\
&\quad +\log(1-x)\mathrm{Li}_2\left(\frac{1-x}{2}\right)-\mathrm{Li}_3\left(\frac{1-x}{2}\right)\ , &(2.84)\\
H(\{-1,-2\};x) &= H(\{-2\};x)\,H(\{-1\};x)-2H(\{-2,-1\};x)\ , &(2.85)\\
H(\{-1,2\};x) &= H(\{-1\};x)\,H(\{2\};x)-H(\{-2,1\};x) \\
&\quad -H(\{2,-1\};x)\ , &(2.86)\\
H(\{-1,1,-1\};x) &= H(\{-1\};x)\,H(\{1,-1\};x)-2H(\{1,-1,-1\};x)\ . &(2.87)
\end{aligned}
$$

### 2.D.3 Weight 4

$$
\begin{aligned}
H(\{1,3\};x) &= -\frac{1}{2}\mathrm{Li}_2(x)^2-\log(1-x)\,\mathrm{Li}_3(x)\ , &(2.88)\\
H(\{1,1,2\};x) &= \frac{1}{2}\log(1-x)^2\,\mathrm{Li}_2(x)+2\log(1-x)\,S_{1,2}(x) \\
&\quad +3S_{1,3}(x)\ , &(2.89)\\
H(\{1,2,1\};x) &= -\log(1-x)\,S_{1,2}(x)-3S_{1,3}(x)\ , &(2.90)\\
H(\{2,2\};x) &= -2S_{2,2}(x)+\frac{1}{2}\mathrm{Li}_2(x)^2\ , &(2.91)\\
H(\{3,1\};x) &= S_{2,2}(x)\ , &(2.92)\\
H(\{2,1,1\};x) &= S_{1,3}(x)\ , &(2.93)\\
H(\{1,1,1,1\};x) &= \frac{1}{24}\log(1-x)^4\ . &(2.94)
\end{aligned}
$$

### 2.D.4 Arbitrary weight

$$
\begin{aligned}
H(\{n\};x) &= \mathrm{Li}_n(x)\,, \qquad n>0\,, &(2.95)\\
H(\{n\};x) &= -\mathrm{Li}_{-n}(-x)\,, \qquad n<0\,, &(2.96)\\
H(\{^n1\};x) &= (-1)^n\frac{\log(1-x)^n}{n!}\ , &(2.97)\\
H(\{^n(-1)\};x) &= \frac{\log(1+x)^n}{n!}\ , &(2.98)\\
H(\{n,^{p-1}1\};x) &= S_{n-1,p}(x)\ . &(2.99)
\end{aligned}
$$

## 2.E HPLs at $i$

In these tables, we collect the values for the HPLs at $i$ up to weight 3.

**Weight 1**

$$H(1;i) = \frac{i\pi}{4} - \frac{\log(2)}{2}\,, \qquad H(-1;i) = \frac{i\pi}{4} + \frac{\log(4)}{4}\,, \tag{2.100}$$

$$H(+;i) = \frac{i\pi}{2}\,, \qquad H(-;i) = -\log(2)\,, \tag{2.101}$$

$$H(0;i) = \frac{i\pi}{2}\,. \tag{2.102}$$

**Weight 2**

$$H(+,i) = \frac{i\pi}{2}\,, \qquad H(-,i) = \log(2)\,, \tag{2.103}$$

$$H(+,-,i) = i\left(2\mathcal{C} - \pi\log(2)\right)\,, \qquad H(-,+,i) = i\left(-2\mathcal{C} + \frac{1}{2}\pi\log(2)\right), \tag{2.104}$$

$$H(0,+,i) = 2i\mathcal{C}\,, \qquad H(0,-,i) = \frac{-\pi}{24}\,, \tag{2.105}$$

$$H(+,0,i) = -2i\mathcal{C} - \frac{\pi^2}{4}\,, \qquad H(-,0,i) = \frac{-\pi}{24} - \frac{i}{2}\pi\log(2)\,. \tag{2.106}$$

**Weight 3**

$$H(+,+,+;i) = -\frac{i\pi^3}{48}\,, \tag{2.107}$$

$$H(+,+,-;i) = \frac{1}{16}\left(\pi^2\log(16) - 21\zeta(3)\right)\,, \tag{2.108}$$

$$H(+,+,0;i) = -\frac{i\pi^3}{16} + \frac{7\zeta(3)}{4}\,, \tag{2.109}$$

$$H(+,-,+;i) = -\mathcal{C}\pi + \frac{21\zeta(3)}{8}\,, \tag{2.110}$$

$$\begin{aligned} H(+,-,-;i) = {} & -\frac{7i\pi^3}{96} - 2i\mathcal{C}\log(2) + \frac{7}{8}i\pi\log^2(2) - 2\mathrm{Li}_3\left(\frac{1}{2} - \frac{i}{2}\right) \\ & + 2\mathrm{Li}_3\left(\frac{1}{2} + \frac{i}{2}\right)\,, \end{aligned} \tag{2.111}$$

$$\begin{aligned} H(+,-,0;i) = {} & -\mathcal{C}\pi + \frac{7i\pi^3}{48} + \frac{1}{2}\pi^2\log(2) + \frac{1}{4}i\pi\log^2(2) + 4\mathrm{Li}_3\left(\frac{1}{2} - \frac{i}{2}\right) \\ & - 4\mathrm{Li}_3\left(\frac{1}{2} + \frac{i}{2}\right)\,. \end{aligned} \tag{2.112}$$

$$H(+,0,+;i) = \mathcal{C}\pi - \frac{7\zeta(3)}{2}, \tag{2.113}$$

$$\begin{aligned} H(+,0,-;i) &= -\frac{11i\pi^3}{96} + 2i\mathcal{C}\log(2) - \frac{1}{8}i\pi\log^2(2) - 2\mathrm{Li}_3\left(\frac{1}{2}-\frac{i}{2}\right) \\ &\quad +2\mathrm{Li}_3\left(\frac{1}{2}+\frac{i}{2}\right), \end{aligned} \tag{2.114}$$

$$H(+,0,0;i) = \mathcal{C}\pi, \tag{2.115}$$

$$H(-,+,+;i) = \mathcal{C}\pi - \frac{1}{8}\pi^2\log(2) - \frac{21\zeta(3)}{16}, \tag{2.116}$$

$$\begin{aligned} H(-,+,-;i) &= \frac{7i\pi^3}{48} + 2i\mathcal{C}\log(2) - \frac{3}{4}i\pi\log^2(2) + 4\mathrm{Li}_3\left(\frac{1}{2}-\frac{i}{2}\right) \\ &\quad -4\mathrm{Li}_3\left(\frac{1}{2}+\frac{i}{2}\right), \end{aligned} \tag{2.117}$$

$$\begin{aligned} H(-,+,0;i) &= \mathcal{C}\pi - \frac{i\pi^3}{32} - \frac{1}{4}\pi^2\log(2) - \frac{1}{8}i\pi\log^2(2) - 2\mathrm{Li}_3\left(\frac{1}{2}-\frac{i}{2}\right) \\ &\quad +2\mathrm{Li}_3\left(\frac{1}{2}+\frac{i}{2}\right), \end{aligned} \tag{2.118}$$

$$\begin{aligned} H(-,-,+;i) &= -\frac{7i\pi^3}{96} + \frac{1}{8}i\pi\log^2(2) - 2\mathrm{Li}_3\left(\frac{1}{2}-\frac{i}{2}\right) \\ &\quad +2\mathrm{Li}_3\left(\frac{1}{2}+\frac{i}{2}\right), \end{aligned} \tag{2.119}$$

$$H(-,-,-;i) = -\frac{1}{6}\log^3(2), \tag{2.120}$$

$$H(-,-,0;i) = \frac{1}{48}\left(12i\pi\log^2(2) - \pi^2\log(4) + 3\zeta(3)\right), \tag{2.121}$$

$$\begin{aligned} H(-,0,+;i) &= -\frac{3i\pi^3}{32} - \frac{1}{8}i\pi\log^2(2) - 2\mathrm{Li}_3\left(\frac{1}{2}-\frac{i}{2}\right) \\ &\quad +2\mathrm{Li}_3\left(\frac{1}{2}+\frac{i}{2}\right), \end{aligned} \tag{2.122}$$

$$H(-,0,-;i) = \frac{1}{24}\left(\pi^2\log(2) - 3\zeta(3)\right), \tag{2.123}$$

$$H(-,0,0;i) = \frac{1}{48}i\left(\pi^3 - 6i\pi^2\log(2) + 9i\zeta(3)\right), \tag{2.124}$$

$$H(0,+,+;i) = -\mathcal{C}\pi + \frac{7\zeta(3)}{4}, \tag{2.125}$$

$$\begin{aligned} H(0,+,-;i) &= -\frac{1}{32}i\left(\pi^3 + 64\mathcal{C}\log(2) + 4\pi\log^2(2)\right) - 2\mathrm{Li}_3\left(\frac{1}{2}-\frac{i}{2}\right) \\ &\quad +2\mathrm{Li}_3\left(\frac{1}{2}+\frac{i}{2}\right), \end{aligned} \tag{2.126}$$

$$H(0,+,0;i) = -\mathcal{C}\pi - \frac{i\pi^3}{8}. \tag{2.127}$$

$$
\begin{aligned}
H(0,-,+;i) &= \frac{1}{8}i\left(\pi^3+2\pi\log^2(2)\right)+4\mathrm{Li}_3\left(\frac{1}{2}-\frac{i}{2}\right) \\
&\quad -4\mathrm{Li}_3\left(\frac{1}{2}+\frac{i}{2}\right) , && (2.128) \\
H(0,-,-;i) &= \frac{\zeta(3)}{16} , && (2.129) \\
H(0,-,0;i) &= -\frac{i\pi^3}{48}+\frac{3\zeta(3)}{8} , && (2.130) \\
H(0,0,+;i) &= \frac{1}{32}i\left(\zeta\left(3,\frac{1}{4}\right)-\zeta\left(3,\frac{3}{4}\right)\right) , && (2.131) \\
H(0,0,-;i) &= -\frac{3\zeta(3)}{16} , && (2.132) \\
H(0,0,0;i) &= -\frac{i\pi^3}{48} . && (2.133)
\end{aligned}
$$

**Arbitrary weight**

$$
\begin{aligned}
H({}^n+;i) &= \frac{(i\pi)^n}{2^n n!} , && (2.134) \\
H({}^n-;i) &= \frac{(-2\log 2)^n}{n!} , && (2.135) \\
H({}^n0;i) &= \frac{(i\pi)^n}{2^n n!} , && (2.136) \\
H({}^n0,+;i) &= i2^{2n+1}\left(\zeta\left(n+1,\frac{1}{4}\right)-\zeta\left(n+1,\frac{3}{4}\right)\right) . && (2.137)
\end{aligned}
$$

The HPLs at $i$ with only 0 and $-$ weights can be converted to HPLs at $x=-1$ using the transformation $x \to x^2$. For weight vectors $s_1,...,s_n$ we have

$$
\begin{aligned}
H(s_1,...,s_n;i) &= H(s'_1,...,s'_n;-1) \\
s_n=-, \quad s_i=0,- \qquad & s'_i = \begin{cases} 1 & s_i=- \\ 0 & s_i=0 , \end{cases} && (2.138)
\end{aligned}
$$

so long as the last element of the weight vector is not a 0. If it is so, one has to extract the 0s from the weight vector, as explained in section 2.2.2.

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# Chapter 3

# Expansion of hypergeometric functions around their parameters

*The first part if this chapter treating the expansion of hypergeometric functions around integer parameters is based on the paper*

*"HypExp, a Mathematica package for expanding hypergeometric functions around integer parameters" [1]*

*published with Tobias Huber in Computer Physics Communications.*

## 3.1 Introduction

As solutions of a large class of differential equations, hypergeometric functions ${}_PF_Q$ appear in many branches of science. They appear, in particular, in particle physics during the calculation of radiative corrections to scattering cross sections in loop [2–7] or phase space [8–10] integrals. In the context of dimensional regularization, the parameters of the hypergeometric functions are usually function of an arbitrary space-time dimension $d = 4 - 2\epsilon$ where $\epsilon$ regulates infrared or ultraviolet divergencies. For physical observables, only the limit $\epsilon \to 0$ is of importance. Because divergencies appear in form of poles $1/\epsilon^n$, not only the constant term of the Taylor expansion is of physical relevance. For this reason one is often confronted with the task of expanding hypergeometric functions around their parameters.

Until recently, there was no systematic approach to the expansion of hypergeometric functions. The required expansions were produced with a case-by-case approach. Recently a general algorithm has been developed [11] for expanding hypergeometric functions with integer parameters and other transcendental functions systematically around their parameters. This algorithm was implemented [12] in the framework of GiNaC [13]. Very recently, a FORM package for expanding transcendental function has become available [14].

In computations involving massive particles [15–21], the hypergeometric functions can have half-integer valued parameters. Methods have been developed to expand hypergeometric functions with half-integer parameters however none of the available (user friendly publicly available) packages was able to perform such an expansion.

In the first section we present one of the algorithms[1] on which the package `HypExp` is based. The second section presents the package itself and the last section presents new developments that allow one to expand hypergeometric functions around half-integer parameters.

## 3.2 HypExp for integer parameters

### 3.2.1 The hypergeometric function

The Gauss hypergeometric function ${}_2F_1(a,b;c;x)$ is defined by

$$ {}_2F_1(a,b;c;x) = 1 + \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{i=1}^{\infty} \frac{\Gamma(a+i)\Gamma(b+i)}{\Gamma(c+i)\Gamma(i+1)} x^i \, , \tag{3.1} $$

it has an integral representation,

$$ {}_2F_1(a,b;c;x) = \frac{\Gamma(c-b)\Gamma(b)}{\Gamma(c)} \int_0^1 t^{b-1}(1-t)^{c-b-1}(1-xt)^{-a}, $$
$$ \mathrm{Re}(c) > \mathrm{Re}(b) > 0, \quad \mathrm{Arg}(1-x) < \pi \, . \tag{3.2} $$

It is the solution of the hypergeometric differential equation

$$ x(1-x)w''(x) + (c-(a+b+1)x)w'(x) - ab\, w(x) = 0 \, . \tag{3.3} $$

The Gauss hypergeometric function ${}_2F_1(a,b;c;z)$ is analytic in $z$ on the complex plane with a branch cut on $(1,\infty)$, it is real on $(0,1)$ and equals 1 at $z=0$.

The generalization of the hypergeometric function is given by

$$ {}_PF_Q(a_1,...,a_P;b_1,...,b_Q;x) = 1 + \frac{\prod_{l=1}^{Q}\Gamma(b_l)}{\prod_{j=1}^{P}\Gamma(a_i)} \sum_{i=1}^{\infty} \frac{\prod_{j=1}^{P}\Gamma(a_j+i)}{\prod_{l=1}^{Q}\Gamma(b_l+i)\Gamma(i+1)} x^i \, , $$

In this chapter we will only be interested in hypergeometric functions with

$$ P = Q + 1. $$

[1] The second algorithm is presented in refs. [1, 22].

### 3.2.2 Nested sums method

In this section, we briefly review $S$ and $Z$ sums and their properties presented in ref. [11], where more detailed derivations can be found.

#### Definitions and auxiliary functions

The definition of the $S$ and $Z$ sums are

$$Z(n, m_{1,\ldots,k}, x_{1,\ldots,k}) = \sum_{i_1=1}^{n} \sum_{i_2=1}^{i_1-1} \cdots \sum_{i_k=1}^{i_{k-1}-1} \frac{x_1^{i_1}}{i_1^{m_1}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}}, \tag{3.4}$$

$$S(n, m_{1,\ldots,k}, x_{1,\ldots,k}) = \sum_{i_1=1}^{n} \sum_{i_2=1}^{i_1} \cdots \sum_{i_k=1}^{i_{k-1}} \frac{x_1^{i_1}}{i_1^{m_1}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}}, \tag{3.5}$$

where we introduced the short-hand notation

$$m_{1,\ldots,k} = \{m_1, \ldots, m_k\}.$$

The number $k$ is called the depth and the sum of the $|m_i|$'s is called the weight of the nested sum. The $S$ and $Z$ sums are related, since their expressions differ only by the upper summation limits in the recursion relation. Using $\sum_{i\leq j} = \sum_{i<j} + \delta_{ij}$, we can convert $S$ into $Z$ sums and vice versa. Due to this possibility, we will in the following concentrate on the $Z$ sums. Similar properties can be derived for $S$ sums [11].

The $Z$ sums of same upper summation index form an algebra, that means that a product of $Z$ sums of a given upper summation index $n$ is expressible as a sum of $Z$ sums of this upper summation index. Since products are defined for equal upper summation limit $n$, it is useful to have a relation between sums $Z(n, \ldots)$ of different $n$'s. The recursive use of the following formulae allows to change the upper summation boundary of a $Z$, and, doing so, to bring all the nested sums to the same upper summation limit. This is called "synchronizing the sums" [11],

$$\begin{aligned} Z(n+c-1, m_{1,\ldots,k}, x_{1,\ldots,k}) &= Z(n-1, m_{1,\ldots,k}, x_{1,\ldots,k}) \\ &+ \sum_{j=0}^{c-1} x_1^j \frac{x_1^n}{(n+j)^{m_1}} Z(n-1+j, m_{2,\ldots,k}, x_{2,\ldots,k}), \end{aligned} \tag{3.6}$$

Since the definition of the $Z$ sums is for denominators of the form $i^{-m}$, it will also be useful to convert sums of the form

$$\sum_{i=1}^{n} \frac{x^i}{(i+c)^m} Z(i-1, \ldots)$$

to the form of the definition, that is, with $c = 0$. If the depth of the sum is zero, we use

$$\sum_{i=1}^{n} \frac{x^i}{(i+c)^m} = \frac{1}{x}\sum_{i=1}^{n} \frac{x^i}{(i+c-1)^m} - \frac{1}{c^m} + \frac{x^n}{(n+c)^m}, \tag{3.7}$$

and otherwise we use

$$\begin{aligned}
&\sum_{i=1}^{n} \frac{x^i}{(i+c)^m} Z(i-1, m_{1,\ldots,k}, x_{1,\ldots,k}) = \\
&\quad \frac{1}{x}\sum_{i=1}^{n} \frac{x^i}{(i+c-1)^m} Z(i-1, m_{1,\ldots,k}, x_{1,\ldots,k}) \\
&\quad -\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m}\frac{x_1^i}{i^{m_1}} Z(i-1, m_{2,\ldots,k}, x_{2,\ldots,k}) \\
&\quad +\frac{x^n}{(n+c)^m} Z(n-1, m_{1,\ldots,k}, x_{1,\ldots,k}).
\end{aligned} \tag{3.8}$$

### Relations to other functions

Special cases of $Z$ and $S$ sums are related to other functions. For infinite upper summation limit, we have the following identities

$$Z(n, \{m_{1,\ldots,k}\}, \{1, ..., 1\}) = Z_{m_1,\ldots,m_k}(n), \tag{3.9}$$

$$Z(\infty, m_{1,\ldots,k}, x_{1,\ldots,k}) = \mathrm{Li}_{m_k,\ldots,m_1}(x_k, \ldots, x_1), \tag{3.10}$$

$$Z(\infty, m_{1,\ldots,k}, 1, \ldots, 1) = \zeta(m_k, \ldots, m_1), \tag{3.11}$$

$$Z(\infty, m_{1,\ldots,k}, \{x, 1, \ldots, 1\}) = H_{m_1,\ldots,m_k}(x), \tag{3.12}$$

$$Z(\infty, \{n+1, \underbrace{1, \ldots, 1}_{p-1}\}, \{x, \underbrace{1, \ldots, 1}_{p-1}\}) = S_{n,p}(x) \quad . \tag{3.13}$$

$Z_{m_1,\ldots,m_k}(n)$ are the Euler-Zagier sums [23, 24], $\mathrm{Li}_{m_k,\ldots,m_1}(x_k, \ldots, x_1)$ are the Goncharov multiple polylogarithms [25]. A special case of the Goncharov multiple polylogarithms are the harmonic polylogarithms (HPL) $H_{m_1,\ldots,m_k}(x)$ of Remiddi and Vermaseren [26]. $\zeta(m_k, \ldots, m_1)$ are the multiple zeta values [27]. The HPLs can be reduced to classical polylogarithms ($\mathrm{Li}_n(x)$) [28] and Nielsen polylogarithms ($S_{n,p}(n)$) [29] up to weight 4 in our case[2]. Because we only have one free variable in the hypergeometric functions, we will only use the last two identities.

The package `HypExp` uses the package `HPL` [30] to deal with harmonic polylogarithms.

[2]For the expansion around integer-valued parameters of the HF, only HPLs with positive indices appear.

**Expansion of the $\Gamma$ function**

$\Gamma$ functions can be expanded around integer values as follows ref. [11]

$$\Gamma(a+\alpha\epsilon) = \Gamma(1+\alpha\epsilon)\Gamma(a)\left(1+\sum_{j=1}^{\infty}(\alpha\epsilon)^j Z_{\underbrace{1,\ldots,1}_{j}}(a-1)\right), \quad (3.14)$$

$$\frac{1}{\Gamma(a+\alpha\epsilon)} = \frac{1}{\Gamma(1+\alpha\epsilon)\Gamma(a)}\left(1+\sum_{j=1}^{\infty}(-\alpha\epsilon)^j S_{\underbrace{1,\ldots,1}_{j}}(a-1)\right), \quad (3.15)$$

for $a$ integer and $a > 0$. For negative (or vanishing) $a$, one has to use the identity $x\Gamma(x) = \Gamma(x+1)$ so that

$$\Gamma(-n+\alpha\epsilon) = \frac{\Gamma(1+\alpha\epsilon)}{\alpha\epsilon}\frac{(-1)^n}{\Gamma(n+1)}\left(1+\sum_{j=1}^{\infty}(\alpha\epsilon)^j S_{\underbrace{1,\ldots,1}_{j}}(n)\right), \quad (3.16)$$

$$\frac{1}{\Gamma(-n+\alpha\epsilon)} = \frac{\alpha\epsilon}{\Gamma(1+\alpha\epsilon)}(-1)^n\Gamma(n+1)\left(1+\sum_{j=1}^{\infty}(-\alpha\epsilon)^j Z_{\underbrace{1,\ldots,1}_{j}}(n)\right). \quad (3.17)$$

**Description of the algorithm**

The algorithm described in this section is the adaptation of the algorithm of type A of ref. [11] for the special case of hypergeometric functions.

The definition of the hypergeometric series is given by

$$\begin{aligned} &{}_JF_{J-1}(\{A_1,\ldots A_J\},\{B_1,\ldots,B_{J-1}\},x) \\ &= 1+\underbrace{\frac{\prod_{l=1}^{Q}\Gamma(b_l)}{\prod_{j=1}^{P}\Gamma(a_i)}}_{E}\underbrace{\sum_{i=1}^{\infty}\frac{\prod_{j=1}^{P}\Gamma(a_j+i)}{\prod_{l=1}^{Q}\Gamma(b_l+i)\Gamma(i+1)}x^i}_{I}. \end{aligned} \quad (3.18)$$

We denote the coefficients in front of the sum with $E$ and the sum itself with $I$. The parameters $A$ and $B$ are of the form

$$A_i = a_i + \alpha_i\epsilon \qquad B_i = b_i + \beta_i\epsilon \qquad a_i, b_i \in \mathbb{Z} \quad \text{and} \quad \alpha_i, \beta_i \in \mathbb{R}\,.$$

In order to give the $\epsilon$-expansion (to order $n$) of the hypergeometric function, one has to expand the product of $E$ and $I$ to order $n$. Let us have a look at the required depth of the $\epsilon$-expansion for these factors.

- For each negative $b_j$, one gets a factor $\epsilon^{-1}$ in $E$, and factors $\epsilon$ in $I$, but only for the values $1,\ldots,-b_j$ of $i$.

- For vanishing $b_j$'s one gets a factor $\epsilon^{-1}$ in $E$ but no factors of $\epsilon$ in $I$.
- For negative $a_j$'s, one gets factors of $\epsilon$ in $E$ and factors $\epsilon^{-1}$ in $I$ for each $i = 1, \ldots, -a_j$,
- For vanishing $a_j$'s, one gets factors of $\epsilon$ in $E$ but no factors $\epsilon^{-1}$ in $I$.

This means that for the expansion of the hypergeometric function to order $n$ we have to compute the expansion of $E$ to order

$$n_E = n + \#(a_j < 0) \tag{3.19}$$

and for $I$ to order

$$n_I = n + \#(b_j \leq 0) - \#(a_j = 0). \tag{3.20}$$

Note that the above argument explains why the expansion of

$$_2F_1(\alpha_1\epsilon, \alpha_2\epsilon, b + \beta\epsilon, x), \qquad b > 0$$

starts with $1 + \mathcal{O}(\epsilon^2)$, whereas that of (for example)

$$_2F_1(1 + \alpha_1\epsilon, 1 + \alpha_2\epsilon, \beta\epsilon, x)$$

has a $\epsilon^{-1}$ term.

We treat first the prefactor

$$E = \frac{\Gamma(B_1) \ldots \Gamma(B_{J-1})}{\Gamma(A_1) \ldots \Gamma(A_J)}. \tag{3.21}$$

We expand the $\Gamma$ functions with the formulae of section 3.2.2, which leads to

$$E = \frac{\Gamma(1 + \beta_1\epsilon) \ldots \Gamma(1 + \beta_{J-1}\epsilon)}{\Gamma(1 + \alpha_1\epsilon) \ldots \Gamma(1 + \alpha_J\epsilon)} f\left(A_1, \ldots, A_J, B_1, \ldots, B_{J-1}, \epsilon\right). \tag{3.22}$$

We have to expand the product of $Z$ sums appearing in $f$ to the order

$$n_E^\Gamma = n_E + \#(b \leq 0) = n + \#(a < 0) + \#(b \leq 0) \tag{3.23}$$

because of the factors $\epsilon^{-1}$ for each negative $b$. Since the factors $\Gamma(1 + \beta_i\epsilon)$ and $\Gamma(1 + \alpha_i\epsilon)^{-1}$ will cancel those coming from the expansion of the $\Gamma$ functions in the sum $I$, we will only consider

$$\begin{aligned} \tilde{E} &= \frac{\Gamma(1 + \alpha_1\epsilon) \ldots \Gamma(1 + \alpha_J\epsilon)}{\Gamma(1 + \beta_1\epsilon) \ldots \Gamma(1 + \beta_{J-1}\epsilon)} \frac{\Gamma(B_1) \ldots \Gamma(B_{J-1})}{\Gamma(A_1) \ldots \Gamma(A_J)} \\ &= f\left(A_1, \ldots, A_J, B_1, \ldots, B_{J-1}, \epsilon\right). \end{aligned} \tag{3.24}$$

The coefficients of the $\epsilon$-expansion of $\tilde{E}$ are $Z$ or $S$ sums with finite upper summation limit. These are rational functions that can be computed easily using the recursive definition.

We now turn to the sum

$$I = \sum_{i=1}^{\infty} \frac{\Gamma(A_1+i)\dots\Gamma(A_J+i)}{\Gamma(B_1+i)\dots\Gamma(B_{J-1}+i)\Gamma(i+1)} x^i \,. \tag{3.25}$$

First one makes use of the identity $x\Gamma(x) = \Gamma(x+1)$ to bring all $\Gamma(A_j+i)$'s and $\Gamma(B_j+i)$'s to the form $\Gamma(i+\xi\epsilon)$ times some rational functions of $i$. Then one expands the $\Gamma$ functions with the formulae of section 3.2.2. As one knows that there will appear terms with, at worst, as many factors $1/\epsilon$ as there are strictly negative $a_j$'s, one has to expand the $\Gamma$-functions to order

$$n_I^\Gamma = n_I + \#(a_j < 0) = n + \#(b_j \le 0) - \#(a_j = 0) + \#(a_j < 0) \tag{3.26}$$

so as to get $I$ to the required order $n_I$. The result of this expansion is a product of

- the factors $\Gamma(1+\xi\epsilon)$ from the expansion of the $\Gamma(i+\xi\epsilon)$. We use them to cancel those from $E$. From now on, we denote by $\tilde{I}$ the sum $I$ without these factors.
- a product of $\epsilon$-expansions with coefficient $Z_{1,\dots,1}(i-1)$ or $S_{1,\dots,1}(i-1)$. These products are treated as above, first converting the $S$ sums into $Z$ sums, then expanding the products of $Z$ sums into a sum of single $Z$ sums. In this case one cannot calculate numerical values for the $Z$ sums, due to the $i$ in the argument.
- a rational function $R(i,\epsilon)$ of $i$ and $\epsilon$ from the factors $x$ in the reduction $x\Gamma(x) = \Gamma(x+1)$. This is reduced by means of expansion into partial fractions to a sum of coefficients times single denominators.

The next step is to bring the factors $1/(i+c)^n$ appearing in $R(i,\epsilon)$ to the form $i^{-m}$ suitable for applying the definition of the $Z$ sums. The method is presented in section 3.2.2.

At this point, one can perform the last summation over $i$, as described in the following section. The result is a sum of $Z$ sums with upper summation limit equal to infinity. These can be converted to more common functions, as described in section 3.2.2.

To obtain the full expansion, one has to multiply the expansions of $\tilde{E}$ and $\tilde{I}$ and to add unity to the result.

### Last summation

The algorithm reduces the sum $\tilde{I}$ to a sum of terms of the form

$$\sum_i x^i \frac{1}{(i+j+\alpha\epsilon)^n} Z\left(i-1, m_{1,\dots,k}, \{1,\dots,1\}\right) .$$

Here we have to distinguish several cases. The general strategy is to perform the summation over $i$ until the denominator is positive for each $i$, then to simplify the remainder to the form of the definition of a $Z$ sum. We list below the different kinds of terms that can appear and for each of them the way it is processed.

- $Z$ sums of argument $i-1$ times one denominator with negative offset:

$$\frac{1}{(i-j+\alpha\epsilon)^m} Z(i-1,\dots).$$

Here one has to perform the sum up to the $j$-th term, using

$$\begin{aligned}
&\sum_{i=1}^{\infty} \frac{1}{(i-j+\alpha\epsilon)^m} Z(i-1,\dots) \\
&= \sum_{k=1}^{j-1} \frac{x^k}{(k-j+\alpha\epsilon)^m} Z(k-1,\dots) + \frac{x^j}{(\alpha\epsilon)^m} Z(j-1,\dots) \\
&\quad + \sum_{k=1}^{\infty} \frac{x^{k+j}}{(k+\alpha\epsilon)^m} Z(k+j-1,\dots)\,.
\end{aligned} \tag{3.27}$$

One then expands the first two terms to the required order in $\epsilon$. The $Z$ sums occurring can be evaluated, as their upper summation limits are finite. We now take a closer look at the last sum

$$\begin{aligned}
&\sum_{k=1}^{\infty} \frac{x^{k+j}}{(k+\alpha\epsilon)^m} Z(k+j-1,\dots) \\
&= x^j \sum_{k=1}^{\infty} x^k \left( \sum_{l=1}^{\infty} (-\alpha\epsilon)^l \frac{1}{k^{l+m}} \frac{(m+l-1)!}{l!(m-1)!} \right) Z(k+j-1,\dots)\,.
\end{aligned} \tag{3.28}$$

Here one only keeps terms up to the required order in $\epsilon$ in the sum over $l$. The $Z$ sum in the last term has to be synchronized down to argument $i-1$, as described in section 3.2.2.

- $Z$ sums of argument $i-1$ times one denominator without offset:

$$\frac{x^i}{i^n} Z(i-1,\dots)\,.$$

If $n$ is positive, following the definition of the $Z$ sums, one gets

$$\sum_i \frac{x^i}{i^n} Z(i-1, m_{2,\dots,k}, \{1,\dots,1\}) = H_{n,m_2,\dots,m_k}(x)\,. \tag{3.29}$$

In many cases, the harmonic polylogarithm can be expressed in terms of more common functions.

If $n$ is negative, one has to interchange the first two summations

$$\begin{aligned}
&\sum_{i=1}^{\infty} i^m x^i Z\left(i-1, m_{2,\ldots,k}, x_{2,\ldots,k}\right) \\
&\quad = \sum_{i_2=1}^{\infty} \frac{x_2^{i_2}}{i_2^{m_2}} Z\left(i_2-1, m_{3,\ldots,k}, x_{3,\ldots,k}\right) \sum_{i=i_2+1}^{\infty} i^m x^i \,. \qquad (3.30)
\end{aligned}$$

The last sum

$$\sum_{i=i_2+1}^{\infty} i^m x^i = \sum_{i=i_2+1}^{\infty} \left(x\frac{\partial}{\partial x}\right)^m x^i = \left(x\frac{\partial}{\partial x}\right)^m \frac{x^{i_2+1}}{1-x} \qquad (3.31)$$

is a polynomial of degree $m$ in $i_2$. The coefficient of each power of $i_2$ is a rational function in $x$. The $i_2^k$ of this polynomial can be combined with the $i_2^{-m_2}$ from the definition of the $Z$-sum. We can also factor out an $x^{i_2+1}$. The remainder is then a polynomial in $i_2$ with rational coefficient functions of $x$. The result is then

$$\begin{aligned}
&\sum_{i=1}^{\infty} i^m x^i Z\left(i-1, m_{2,\ldots,k}, x_{2,\ldots,k}\right) \\
&\quad = x\sum_{i_2=1}^{\infty} \frac{(x x_2)^{i_2}}{i_2^{m_2}} Z\left(i_2-1, m_{3,\ldots,k}, x_{3,\ldots,k}\right) \sum C_j(x) i_2^j \,. \qquad (3.32)
\end{aligned}$$

We are now left over with a sum of terms of the form

$$C(x)\sum_{i_2=1}^{\infty} \frac{(x x_2)^{i_2}}{i_2^{\tilde{m}}} Z\left(i_2-1, m_{3,\ldots,k}, x_{3,\ldots,k}\right).$$

Recursive use of this formula leads either to $Z$ sums with a denominator with positive $\tilde{m}$ or to a $Z$ sum multiplied by a denominator with negative exponent $n$ but with zero depth. For the latter we can apply

$$\sum_{i=1}^{\infty} x^i i^m Z\left(i-1, \{\}, \{\}\right) = \sum_{i=1}^{\infty} x^i i^m = \mathrm{Li}_{-m}(x) = \left(x\frac{\partial}{\partial x}\right)^m \frac{x}{1-x}\,, \qquad (3.33)$$

which is also a rational function in $x$.

- $Z$ sums of argument $i-1$ without denominators:

$$x^i Z(i-1, m_{2,\ldots,k}, \{1,\ldots,1\})\,.$$

The summation can be performed by exchanging the first two summations

$$\sum_{i=1}^{\infty} x^i Z(i-1, m_{2,\ldots,k}, \{1,\ldots,1\}) = \frac{x}{1-x} H_{m_2,\ldots}(x) \tag{3.34}$$

- Single denominator with negative offset:

$$\sum_i \frac{x^i}{(i-j+\alpha\epsilon)^m} \, .$$

Here we perform the sum explicitly for the $j$ first terms

$$\sum_{i=1}^{\infty} \frac{x^i}{(i-j+\alpha\epsilon)^m} = \sum_{k=1}^{j-1} \frac{x^k}{(k-j+\alpha\epsilon)^m} + \frac{x^j}{(\alpha\epsilon)^m} + x^j \sum_{k=1}^{\infty} \frac{x^k}{(k+\alpha\epsilon)^m}, \tag{3.35}$$

we can simplify the last summation if we are only interested in the expansion to order $n$:

$$\sum_{k=1}^{\infty} \frac{x^k}{(k+\alpha\epsilon)^m} = \sum_{l=0}^{n} \frac{(m+l-1)!}{l!(m-1)!} (-\alpha\epsilon)^l \mathrm{Li}_{m+l}(x) + O(\epsilon^{n+1}) \, . \tag{3.36}$$

Note that this works for positive and negative $m$.

- Single denominator with positive offset:

$$\sum_i \frac{x^i}{(i+j)^m} \, .$$

We use the formula

$$\sum_{i=1}^{\infty} \frac{x^i}{(i+j)^m} = \frac{1}{x^j} \left( \mathrm{Li}_m(x) - \sum_{i=1}^{j} \frac{x^i}{i^m} \right) \, . \tag{3.37}$$

## 3.3 The Mathematica implementation `HypExp`

We implemented the results of the previous section in the `Mathematica` package `HypExp`. It allows one to expand arbitrary ${}_JF_{J-1}$-functions to arbitrary order in a small quantity around integer parameters. It can be obtained from link [31]. The results are displayed in terms of rational functions, logarithms, polylogarithms, Nielsen polylogarithms, and harmonic polylogarithms. The results given by these functions are not systematically simplified using `Simplify`, since the simplification might take longer than the expansion itself, in particular for expansions to high orders. Use of `Simplify` might produce a more compact result.

After installation[3], the package `HypExp` may be loaded using the following command,

```
<< HypExp`
```

This should be done at the beginning of the session.

### 3.3.1 Functions, commands and symbols added

The package `HypExp` adds two new symbols

- `$HypExpPath` is the path where the `HypExp` package is installed.
- `$HypExpFailed` is the symbol returned by the package in case of failure.

The package adds the following functions

- `HypExp[Hypergeometric2F1[...,x],`$\epsilon$`,n]` gives the $\epsilon$ expansion of the enclosed hypergeometric function (HF). The function `HypExp` applied to anything else but a HF will leave it intact. Therefore one can map it onto an expression containing hypergeometric functions, and only the HF will be expanded to the required order in $\epsilon$. This is illustrated by the following example:

```
(HypExp[#1, ϵ, 1] &) //@
 (Log[1 - ϵ] Hypergeometric2F1[1 + ϵ, 1, 2 - ϵ, x])
```

$$\mathrm{Log}[1-\epsilon]\left(-\frac{\mathrm{Log}[1-x]}{x}+\epsilon\left(\frac{\mathrm{Log}[1-x]}{x}+\frac{\mathrm{Log}[1-x]^2}{x}+\frac{\mathrm{PolyLog}[2,x]}{x}\right)\right)$$

```
(HypExp[#1, ϵ, 1] &) //@ (Log[1 - ϵ]
   HypergeometricPFQ[{1 + 2 ϵ, 1 - ϵ, 2}, {2 - ϵ, 2 + 3 ϵ}, x])
```

$$\mathrm{Log}[1-\epsilon]\left(-\frac{\mathrm{Log}[1-x]}{x}+\epsilon\left(-\frac{2\,\mathrm{Log}[1-x]}{x}-\frac{\mathrm{Log}[1-x]^2}{2x}-\frac{2\,\mathrm{PolyLog}[2,x]}{x}\right)\right)$$

```
Simplify[%]
```

$$-\frac{1}{2x}(\mathrm{Log}[1-\epsilon](\mathrm{Log}[1-x](2+4\epsilon+\epsilon\,\mathrm{Log}[1-x])+4\epsilon\,\mathrm{PolyLog}[2,x]))$$

The result is not returned as a `SeriesData` object because this would have the effect of forcing the expansion of the rest of the expression. This example also illustrates the absence of automatic simplification of the results produced by the package, as this might be time consuming and not always appropriate. If one wants to get a compact result, one should use `Simplify` or even `FullSimplify`. The prefactors that accompany the variable $\epsilon$ can also be symbolic, and the expansion also works for argument $z = 1$ as shown

[3] see link [31] for more information on the installation procedure

by the following example,

```
FullSimplify[HypExp[
  Hypergeometric2F1[1 + 3 ϵ, 1 - 2 ϵ, 3 + 2 ϵ, 1], ϵ, 4]]
```

$$\frac{1}{3}\left(6-6\left(-6+\pi^2\right)\epsilon^2-\left(-468+36\pi^2+\pi^4\right)\epsilon^4+108\epsilon^3\left(-1+\text{Zeta}[3]\right)\right)$$

```
HypExp[HypergeometricPFQ[
  {1 + ϵ, 1 - 2 ϵ, 2 - 3 ϵ}, {2 + 2 ϵ, 2 - ϵ}, 1], ϵ, 2]
```

$$\frac{4}{5}+\frac{1}{5\epsilon}+\left(2-\frac{2\pi^2}{5}\right)\epsilon+\epsilon^2\left(6-\frac{8\pi^2}{5}+\frac{78\,\text{Zeta}[3]}{5}\right)$$

The technicalities of the expansion in the case of the argument being unity are explained in refs. [1, 22].

- The relations (3.115) – (3.138) between polylogarithms $\mathrm{Li}_n$ and Nielsen polylogarithms $S_{n,p}$ of different arguments listed in appendix 3.A.1 are used internally. By setting the constant `$HypExpPolyLogRules` to `True`, these identities are applied systematically. Its default value is `False`. This is also illustrated with an example,

```
$HypExpPolyLogRules = False;
PolyLog[2, z/(z - 1)]
```

$$\text{PolyLog}\left[2,\frac{z}{-1+z}\right]$$

```
$HypExpPolyLogRules = True;
PolyLog[2, z/(z - 1)]
```

$$-\frac{1}{2}\text{Log}[1-z]^2-\text{PolyLog}[2,z]$$

- The function `HypExpInt`$[\chi_1, \chi_2, \chi_3, \chi_4, \chi_5, z]$ evaluates integrals of the form

$$I\left(\chi_1,\chi_2,\chi_3,\chi_4,\chi_5,z\right):=\int_0^1 du\,\frac{u^{\chi_1}\ln^{\chi_2}(u)\ln^{\chi_3}(1-u)\ln^{\chi_4}(1-zu)}{(uz-1)^{\chi_5}}\,,\quad(3.38)$$

with

$$w=\chi_2+\chi_3+\chi_4+1-\delta_{\chi_5,0}\leq 5\,.$$

The algorithms for these integrals are explained in refs. [1, 22]. All the $\chi_i$ are non-negative integers and $z\in\mathbb{C}\backslash(1,\infty)$. The upper bound on the weight $w$ stems from the fact that the expansion of ${}_2F_1$-functions up to order $\mathcal{O}(\epsilon^4)$ also involves integrals of weight 5. The integral can be called with the argument being symbolic:

```
HypExpInt[2, 0, 1, 1, 3, z]
```

$$\frac{\left(27+2\pi^2-24z-4\pi^2z+2\pi^2z^2\right)\text{Log}[1-z]}{12\,(-1+z)^2z^3}-\frac{(-3+4z)\,\text{Log}[1-z]^2}{2\,(-1+z)^2z^3}+\frac{\text{Log}[1-z]^3}{3z^3}-\frac{\text{Log}[1-z]^2\,\text{Log}[z]}{2z^3}-\frac{(-3+4z)\,\text{PolyLog}[2,z]}{2\,(-1+z)^2z^3}-\frac{\text{PolyLog}[3,1-z]}{z^3}+\frac{3z+4\,\text{Zeta}[3]-8z\,\text{Zeta}[3]+4z^2\,\text{Zeta}[3]}{4\,(-1+z)^2z^3}$$

Arguments that match the pattern $z/(z-1)$ are treated using the relations between polylogarithms of different arguments, appendix 3.A.1 (if `$HypExpPolyLogRules` is set to `True`):

```
HypExpInt[1, 1, 0, 1, 2, z/(z - 1)]
-((6 + π^2) (-1 + z)^2 Log[1 - z])/(6 z^2) + ((-1 + z)^2 Log[1 - z]^3)/(6 z^2) +
 ((-1 + z)^2 Log[1 - z]^2 Log[z])/(2 z^2) - ((-1 + z)^2 PolyLog[2, z])/z^2 +
 ((-1 + z)^2 Log[1 - z] PolyLog[2, z])/z^2 +
 ((-1 + z)^2 PolyLog[3, 1 - z])/z^2 - ((-1 + z)^2 Zeta[3])/z^2
```

Finally, also all $z \in \mathbb{C}/(1,\infty)$ can be inserted directly. For the special cases $z = 0$ and $z = 1$ the integral simplifies considerably and the restriction $w \leq 5$ can be dropped.

```
HypExpInt[2, 4, 1, 1, 3, 1]
3 π^4/2 + π^6/6 - 42 Zeta[3] + 22 π^2 Zeta[3] + 2/3 π^4 Zeta[3] -
 108 Zeta[3]^2 - 348 Zeta[5] + 16 π^2 Zeta[5] - 240 Zeta[7]
```

In the case $z = 1$ we refer the reader also to the next paragraph.

- The function `HypExpU`$[n, m, p]$ gives the result of the definite integral

$$U(n,m,p) := \int_0^1 du \ln^n(u) \cdot \ln^m(1-u) \cdot u^p \ , \tag{3.39}$$

with $p \in \mathbb{Z}$ and $n$, $m$ being non-negative integers. In order to yield a convergent integral the inequality $m+p \geq 0$ has to be satisfied. The algorithm to compute this integrals is described in refs. [1, 22].

```
HypExpU[4, 3, -2]
2 π^4 + π^6/3 - 144 Zeta[3] + 48 π^2 Zeta[3] + 18/5 π^4 Zeta[3] -
 216 Zeta[3]^2 - 576 Zeta[5] + 72 π^2 Zeta[5] - 1152 Zeta[7]
```

- `HypExpIsKnownToOrder`$[a_1, \ldots, a_J\ , b_1, \ldots, b_{J-1}, n]$ returns `True` if the expansion of the hypergeometric function with parameters corresponding to the first arguments of the function is available in the library to the order $n$.

- `HypExpAddToLib` adds an expansion to the library. This function is described in section 3.3.3.

### 3.3.2 Functions modified

The package also updates `Series` to allow it to expand compound expressions containing hypergeometric functions. The difference between this and the mapping with `HypExp` is that the other functions of $\epsilon$ are also expanded, as shown by the following example:

```
Series[
 Log[1 - ϵ] Hypergeometric2F1[ϵ + 1, 1, 2 - ϵ, x], {ϵ, 0, 2}]
```

$$\frac{\text{Log}[1-x]\,\epsilon}{x} + \left(-\frac{\text{Log}[1-x]}{2\,x} - \frac{\text{Log}[1-x]^2}{x} - \frac{\text{PolyLog}[2,x]}{x}\right)\epsilon^2 + O[\epsilon]^3$$

```
Series[Log[1 - ϵ] HypergeometricPFQ[
   {2 ϵ + 1, 1 - ϵ, 2}, {2 - ϵ, 3 ϵ + 2}, x], {ϵ, 0, 2}]
```

$$\frac{\text{Log}[1-x]\,\epsilon}{x} + \left(\frac{5\,\text{Log}[1-x]}{2\,x} + \frac{\text{Log}[1-x]^2}{2\,x} + \frac{2\,\text{PolyLog}[2,x]}{x}\right)\epsilon^2 + O[\epsilon]^3$$

This allows to work with the expansion of HFs as `Mathematica` users are used to. We also updated the series expansion of the regularized hypergeometric functions since they are nothing else but hypergeometric functions divided by $\Gamma$-functions.

As the incomplete $B$ function is a special case of an HF,

$$B(z,a,b) = \frac{z^a}{a}\,{}_2F_1(a, 1-b, a+1, z), \quad a \neq -1, -2, \ldots \qquad , \tag{3.40}$$

it is also possible to expand it with the method described in this paper. Therefore we also updated the series expansion of the incomplete $B$ function around integer values of its parameters, as shown by the following example.

```
Series[Beta[x, 1 + 2 ϵ, 2 - ϵ], {ϵ, 0, 1}]
```

$$\left(x - \frac{x^2}{2}\right) + \left(-\frac{3\,x}{2} + \frac{x^2}{4} + \frac{1}{2}\,\text{Log}[1-x] - x\,\text{Log}[1-x] + \frac{1}{2}\,x^2\,\text{Log}[1-x] + 2\,x\,\text{Log}[x] - x^2\,\text{Log}[x]\right)\epsilon + O[\epsilon]^2$$

### 3.3.3 Working with the libraries

Since the computation of the expansion for high orders and large parameters is quite time consuming, it is of interest to store the results that have been already calculated and reuse them, instead of recalculating them. The `HypExp` library contains expansions of HFs for some sets of parameters. When an expansion is requested, the package first checks whether the library contains the expansion for the requested set of parameters to the requested order. If so, it loads it and gives the answer, if not, it proceeds with the calculation along the line of the preceding sections. The library management can be called dynamic in the sense that elements of the library are loaded in the memory at run time only if they are needed.

The package HypExp has a standard library. Further libraries can be added, depending on the needs and on the amount of available disk space. The different libraries can be found at link [31].

The package also allows extending the provided libraries with HFs not included in the standard libraries, or included but not to a sufficiently high expansion order. The expansion of ${}_JF_{J-1}(a_1,\ldots,a_J,b_1,\ldots,b_{J-1},x)$ to order $n$ can be added to the library with the command

HypExpAddToLib[$a_1$,...,$a_J$,$b_1$,...,$b_{J-1}$,n]

where $a_1,\ldots,a_j,b_1,\ldots,b_{J-1}$ are integers. At this command, Mathematica will compute the expansion for arbitrary $\epsilon$-parts added to the integers $a_1,\ldots,a_J$ and $b_1,\ldots,b_{J-1}$. As arbitrary coefficients are more difficult than numbers, the time needed to add an expansion to the library is longer than the time for a single evaluation. Therefore adding expansions to the library is only useful if this expansion shows up repeatedly. The result is then saved in the library in the installation directory, so that it can be used in future Mathematica sessions. As the results are supposed to be used several times, the result of the expansion is simplified using Simplify, in order to get a more compact result. This, in turn, makes the extension of the library even more time consuming.

The library files are copied to the installation directory of the package[4] during the installation. Further libraries can be added as described at link [31].

Due to our naming conventions for the entries in the library files, the expansions of HFs of parameters higher in absolute value than 9 are not allowed.

### 3.3.4 Note on the expansion for negative parameters

Let us consider ${}_2F_1(-m+\alpha,-b,-m-l+\beta;x)$ for $m$, $l$, $b$ positive integers, $b>m$ and $\alpha$, $\beta$ small. Using the definition one gets

$$ {}_2F_1(-m+\alpha,-b,-m-l+\beta;x)=\sum_{n=0}^{\infty}\frac{(-m+\alpha)_n(-b)_n}{(-l-m+\beta)_n n!}x^n\ . \tag{3.41}$$

We are interested in the terms for $n$ between $m$ and $b$. All further terms vanish, since then $(-b)_n$ becomes 0. They are equal to

$$\frac{(-m+\alpha)\ldots(1+\alpha)\alpha(-b)(1-b)\ldots(m-b)}{(-m+\beta-l)(-m+\beta+1-l)\ldots(1+\beta-l)(\beta-l)}x^m+\cdots+ \\ \frac{(-m+\alpha)\ldots\alpha(1+\alpha)\ldots(m-b+\alpha)(-b)\ldots(-b+m+l)}{(-m+\beta-l)\ldots(1+\beta)\beta}x^{m+l}+\ldots \tag{3.42}$$

[4]which is stored in the Mathematica variable \$HypExpPath

If one wants to define a value for ${}_2F_1(-m,-b,-m-l;x)$ one has to take the limit of the above expression for $\alpha$ and $\beta$ going to zero. The result depends on the way one approaches $(0,0)$ with $\alpha$ and $\beta$. In ref. [32], one can find the formula

$$ {}_2F_1(-m,b,-m-l;x) = \sum_{n=0}^{\infty} \frac{(-m)_n (b)_n}{(-l-m)_n n!} x^n \,, \tag{3.43} $$

which is also the result `Mathematica` gives. This corresponds to a trajectory in the $(\alpha,\beta)$-plane going along the $\beta$ axis. Taking a trajectory along the $\alpha$ axis would lead to a $1/\beta$ pole. Any other trajectory gives a constant times a function. This function happens to be the second solution of the differential equation satisfied by ${}_2F_1(-m+\alpha,-b,-m-l+\beta;x)$,

$$ x(1-x)\,w''(x) + (B_1 - (A_1+A_2+1)x)\; w'(x) - A_1\,A_2\,w(x) = 0 \,, \tag{3.44} $$

with

$$ A_1 = -m+\alpha\,, \qquad A_2 = -b\,, \qquad B_1 = -m-l+\beta\,. \tag{3.45} $$

In the case of negative or vanishing $c$, the value at $x=0$ of this function is also equal to unity. This prevents us from discriminating between the two solutions by their values at $x=0$.

Since the use of the Kummer identity

$$ {}_2F_1(A_1,A_2;B_1;x) = (1-x)^{B_1-A_1-A_2}\,{}_2F_1(B_1-A_1,B_1-A_2;B_1;x) \tag{3.46} $$

induces a rotation in the $(\alpha,\beta)$ plane and since `Mathematica` always chooses the trajectory along the $\beta$ axis, the result for the HF and its Kummer transform will not be identical in `Mathematica` for this particular case.

### 3.3.5 Performance and limitations

Performance limits are set by the CPU and the amount of memory available. In all practical cases known to the author, however, the result is given in a reasonable time. The following table shows the CPU time dependence for the expansion of some hypergeometric functions to different orders on a 3 GHz processor/1.5 GB RAM machine.

| order | 2 | 3 | 4 | 5 |
|---|---|---|---|---|
| ${}_2F_1(1+\epsilon,1-\epsilon;2+2\epsilon,x)$ | $<1$ s | $<1$ s | $<1$ s | 7 s |
| ${}_2F_1(1+\alpha_1\epsilon,1+\alpha_2\epsilon;2+\beta_1\epsilon,x)$ | $<1$ s | $<1$ s | $<1$ s | 6 s |
| ${}_3F_2(1+2\epsilon,1-\epsilon,2-3\epsilon;1+3\epsilon,2+\epsilon,x)$ | $<1$ s | $<1$ s | $<1$ s | 3 s |
| ${}_3F_2(1+\alpha_1\epsilon,1+\alpha_2\epsilon,2+\alpha_3\epsilon;$ $1+\beta_1\epsilon,2+\beta_2\epsilon,x)$ | $<1$ s | $<1$ s | 1.5 s | 3 s |
| ${}_4F_3(1+\alpha_1\epsilon,2+\alpha_2\epsilon,3+\alpha_3\epsilon,4+\alpha_4\epsilon;$ $\beta_1\epsilon,1+\beta_2\epsilon,1+\beta_3\epsilon,x)$ | 12 s | 20 s | 50 s | 140 s |

This package was developed in `Mathematica 5.0` and should also work on newer versions.

## 3.4 HypExp for half-integer parameters

In this section we describe an algorithm to expand hypergeometric functions about half-integer parameters.

### 3.4.1 Definitions and notation

In this section we introduce some definitions and notation that will be used in the following sections. In this paper we consider hypergeometric functions (hereafter HF)

$$ {}_PF_{P-1}(A_1, ..., A_P; B_1, ..., B_{P-1}; z) $$

whose parameters $A_j$ and $B_j$ have the following form

$$ i + \gamma\epsilon \quad \text{or} \quad i + \frac{1}{2} + \gamma\epsilon \; , $$

where $i$ is an integer, $\gamma$ is a real coefficient and $\epsilon$ is the parameter in which we will expand the HF.

We will denote the finite part (i.e. either $i$ or $i + \frac{1}{2}$) of a parameter by lower case Latin letters, the coefficients of the expansion parameter $\epsilon$ will be labelled by Greek $\alpha$ or $\beta$ and the whole parameter will be referred to by capital $A$ or $B$. $A$, $a$ and $\alpha$ always correspond to an element of the first subset of argument whereas $B$, $b$ and $\beta$ correspond to the second subset of parameters.

We will refer to an HF as being of the type $P^i_j$ if $i$ out of the $P$ $a_k$s, $j$ out of the $P-1$ $b_k$s are half-integers and the other $a_k$s and $b_k$s are integers.

We define the short-hand notation

$$ \prod_j^{a:a} = 1, \quad \prod_j^{a:b} f(j) = \prod_{j=a}^{b-1} f(j) \quad \text{if} \quad a < b, \quad \prod_j^{a:b} f(j) = \prod_{j=b}^{a-1} \frac{1}{f(j)} \quad \text{if} \quad a > b \; , \tag{3.47} $$

so that

$$ \Gamma(b) = \Gamma(a) \prod_j^{a:b} (j) \; . $$

### 3.4.2 Algorithm

The algorithm is based on the fact that one can write fractions of the type

$$ \frac{x^i}{(i+j)^n} $$

with $i+j \neq 0$ in terms of the integration operator

$$J^+(j)[f](x) = \frac{1}{x^j}\int_0^x \mathrm{d}x' x'^{j-1} f(x') \equiv J^+(j,1)[f](x), \tag{3.48}$$

$$J^+(j,n)[f](x) \equiv \left(J^+(j)\right)\left[J^+(j,n-1)[f]\right](x) \tag{3.49}$$

in the following way

$$\frac{x^i}{i+j} = \frac{1}{x^j}\int_0^x \mathrm{d}x' x'^{j-1} x'^i \equiv J^+(j)[y^i](x), \tag{3.50}$$

$$\frac{x^i}{(i+j)^n} \equiv J^+(j,n)[y^i](x)\ . \tag{3.51}$$

Polynomials in $i$ and $x$ can also be written using

$$i x^i = x\frac{\mathrm{d}}{\mathrm{d}x}x^i, \qquad i^j x^i = \left(x\frac{\mathrm{d}}{\mathrm{d}x}\right)^j x^i\ ,$$

for which we define the operator

$$J^-(j)[f](x) = \frac{1}{x^{j-1}}\frac{\mathrm{d}}{\mathrm{d}x}x^j f(x)\ . \tag{3.52}$$

In the following we will illustrate the algorithm with an HF of type $2^1_1$.

### Hypergeometric functions of type $2^1_1$

We start from the definition of the Hypergeometric function ${}_2F_1$

$${}_2F_1(A_1,A_2,B_1,x) = 1 + \frac{\Gamma(B_1)}{\Gamma(A_1)\Gamma(A_2)}\sum_{i=1}^{\infty}\frac{\Gamma(A_1+i)\Gamma(A_2+i)}{\Gamma(B_1+i)\Gamma(i+1)}x^i\ . \tag{3.53}$$

We consider the case where the finite part of $A_1$ and $B_1$ are half-integers and that of $A_2$ is an integer

$$A_1 = a_1 + \frac{1}{2} + \alpha_1\epsilon, \quad A_2 = a_2 + \alpha_2\epsilon, \quad B_1 = b_1 + \frac{1}{2} + \beta_1\epsilon\ .$$

Using the relation $x\Gamma(x) = \Gamma(x+1)$ we can transform this expression (3.53) into

$$
\begin{aligned}
&{}_2F_1(a_1 + \frac{1}{2} + \alpha_1\epsilon, a_2 + \alpha_2\epsilon, b_1 + \frac{1}{2} + \beta_1\epsilon, x) = \\
&= \quad 1 + \frac{\Gamma(\frac{1}{2}+\beta_1\epsilon)}{\Gamma(\frac{1}{2}+\alpha_1\epsilon)\Gamma(1+\alpha_2\epsilon)} \frac{\prod_j^{0:b_1}(j+\frac{1}{2}+\beta_1\epsilon)}{\prod_j^{0:a_1}(j+\frac{1}{2}+\alpha_1\epsilon)\prod_j^{1:a_2}(j+\alpha_2\epsilon)} \\
&\times \quad \sum_{i=1}^{\infty} \underbrace{\frac{\prod_j^{0:a_1}(i+j+\frac{1}{2}+\alpha_1\epsilon)\prod_j^{1:a_2}(i+j+\alpha_2\epsilon)}{\prod_j^{0:b_1}(i+j+\frac{1}{2}+\beta_1\epsilon)}}_{D} \frac{\Gamma(i+\frac{1}{2}+\alpha_1\epsilon)\Gamma(i+1+\alpha_2\epsilon)}{\Gamma(i+\frac{1}{2}+\beta_1\epsilon)\Gamma(i+1)} x^i \,.
\end{aligned}
\tag{3.54}
$$

Where we made use of the short-hand notation defined in (3.47). The factor $D$ in (3.54) can be turned into partial fractions with respect to $i$. This yields a sum of factors $i^n$, $1/(i+j+\gamma\epsilon)^n$ or $1/(i+j+1/2+\gamma\epsilon)^n$ .

$$
\begin{aligned}
&{}_2F_1(a_1 + \frac{1}{2} + \alpha_1\epsilon, a_2 + \alpha_2\epsilon, b_1 + \frac{1}{2} + \beta_1\epsilon, x) = \\
&= \quad 1 + \frac{\prod_j^{0:b_1}(j+\frac{1}{2}+\beta_1\epsilon)}{\prod_j^{0:a_1}(j+\frac{1}{2}+\alpha_1\epsilon)\prod_j^{1:a_2}(j+\alpha_2\epsilon)} \frac{\Gamma(\frac{1}{2}+\beta_1\epsilon)}{\Gamma(\frac{1}{2}+\alpha_1\epsilon)\Gamma(1+\alpha_2\epsilon)} \\
&\quad \times \sum_{i=1}^{\infty} \left( \sum_{j\geq 0,n} \frac{C^+_{j,n}}{(i+j+\gamma\epsilon)^n} + \sum_{j<0,n} \frac{C^+_{j,n}}{(i+j+\gamma\epsilon)^n} \right. \\
&\qquad\qquad \left. + \sum_{j,n} \frac{C^{1/2}_{j,n}}{(i+\frac{1}{2}+j+\gamma\epsilon)^n} + \sum_n C^-_n i^n \right) \\
&\quad \times \frac{\Gamma(i+1+\alpha_1\epsilon)\Gamma(i+\frac{1}{2}+\alpha_2\epsilon)}{\Gamma(i+\frac{1}{2}+\beta_1\epsilon)\Gamma(i+1)} x^i \,,
\end{aligned}
\tag{3.55}
$$

where the coefficients $C_j$ and $C_j^{1/2}$ are polynomials in $\epsilon$. The sum over positive $j$'s can be expanded in $\epsilon$ which yields factors of $1/(i+j)^n$ that can be expressed as integration operators

$$
J^+(j,n) = \left( \frac{1}{x^j} \int_0^x \mathrm{d}x' x'^{j-1} \right)^n \tag{3.56}
$$

acting on

$$B \equiv \frac{\Gamma(\frac{1}{2}+\beta_1\epsilon)}{\Gamma(\frac{1}{2}+\alpha_1\epsilon)\Gamma(1+\alpha_2\epsilon)} \sum_{i=1}^{\infty} \frac{\Gamma(i+\frac{1}{2}+\alpha_1\epsilon)\Gamma(i+1+\alpha_2\epsilon)}{\Gamma(i+\frac{1}{2}+\beta_1\epsilon)\Gamma(i+1)} x^i$$
$$= {}_2F_1(\frac{1}{2}+\alpha_1\epsilon, 1+\alpha_2\epsilon, \frac{1}{2}+\beta_1, x) - 1 \, . \tag{3.57}$$

The same applies for the terms of the form $1/(i+\frac{1}{2}+j+\gamma\epsilon)^n$ with the integration operator

$$J^+_{1/2}(j,n) = \left( \frac{1}{x^{j+\frac{1}{2}}} \int_0^x \mathrm{d}x' x'^{j-\frac{1}{2}} \right)^n = J^+(j+\frac{1}{2}, n) \, .$$

The factors $i^n$ can be written as differentiation operators

$$J^-(n) = \left( x\frac{\mathrm{d}}{\mathrm{d}x} \right)^n \tag{3.58}$$

acting on $B$. For the terms with $j = -k < 0$ we decompose the sum over $i$ in three parts, one running from 1 to $k-1$, the term $i = k$ and the remaining sum to infinity

$$\sum_{i=1}^{\infty} \frac{x^i}{(i-k+\gamma\epsilon)^n} B_i = \sum_{i=1}^{k-1} \frac{x^i}{(i-k+\gamma\epsilon)^n} B_i + \frac{x^k}{(\gamma\epsilon)^n} B_k + \sum_{i=k+1}^{\infty} \frac{x^i}{(i-k+\gamma\epsilon)^n} B_i \, . \tag{3.59}$$

The last term can be worked out as follows

$$\sum_{i=k+1}^{\infty} \frac{x^i}{(i-k+\gamma\epsilon)^n} B_i$$
$$= \sum_{i=1}^{\infty} \frac{x^i x^k}{(i+\gamma\epsilon)^n} B_{i+k} = x^k \sum_{i=1}^{\infty} \frac{x^i}{(i+\gamma\epsilon)^n} B_{i+k} \tag{3.60}$$
$$= x^k \sum_{l=0}^{\infty} \frac{(n+l-1)!}{l!(n-1)!} (-\gamma\epsilon)^l \sum_{i=1}^{\infty} \frac{x^i}{(i)^{n+l}} B_{i+k}$$
$$= x^k \sum_{l=0}^{\infty} \frac{(n+l-1)!}{l!(n-1)!} (-\gamma\epsilon)^l \left[ J^+(0, n+l) \right] \left( \sum_{i=1}^{\infty} x^{-k} x^i \tilde{B}_{i,k} \right)$$
$$= x^k \sum_{l=0}^{\infty} \frac{(n+l-1)!}{l!(n-1)!} (-\gamma\epsilon)^l \left[ J^+(0, n+l) \right] \left( x^{-k} \tilde{B}(k,x) \right) \, , \tag{3.61}$$

where

$$\tilde{B}_{i,k} = \begin{cases} 0, & i \leq k \\ B_i, & i > k \end{cases} \qquad \text{and} \qquad \tilde{B}(k,x) = \sum_{i=1}^{\infty} x^i \tilde{B}_{i,k} \, . \tag{3.62}$$

One can now write the terms with $j<0$ in $D$ as an operator

$$
\begin{aligned}
&\frac{1}{(i-j+\gamma\epsilon)^n} \to J^+(j,n,\gamma)B \\
&\equiv \sum_{i=1}^{j} \frac{B_i x^i}{(i-j+\gamma\epsilon)^n} + x^j \sum_{l=0}^{\infty} \frac{(n+l-1)!}{l!(n-1)!}(-\gamma\epsilon)^l J^+(0,n+l)\left(x^{-j}\tilde{B}(j)\right) ,
\end{aligned}
\tag{3.63}
$$

where $B_i$ is the $i$-th coefficient of the Taylor expansion in $x$ of $B$ about $x=0$

$$
B_i = \frac{\Gamma(a_1+\frac{1}{2}+i+\alpha_1\epsilon)\Gamma(a_2+1+i+\alpha_2\epsilon)\Gamma(b_1+\frac{1}{2}+\beta_1\epsilon)}{\Gamma(a_1+\frac{1}{2}+\alpha_1\epsilon)\Gamma(a_2+1+\alpha_2\epsilon)\Gamma(b_1+\frac{1}{2}+i+\beta_1\epsilon)i!} , \tag{3.64}
$$

The final formula reads

$$
{}_2F_1(a_1+\frac{1}{2}+\alpha_1\epsilon, a_2+\alpha_2\epsilon, b_1+\frac{1}{2}+\beta_1\epsilon, x) \tag{3.65}
$$

$$
\begin{aligned}
&= 1+\frac{\prod_j^{0:b_1}(j+\frac{1}{2}+\beta_1\epsilon)}{\prod_j^{0:a_1}(j+\frac{1}{2}+\alpha_1\epsilon)\prod_j^{1:a_2}(j+\alpha_2\epsilon)} \\
&\times \left(\sum_{j\geq 0,n} C^+_{j,n} J^+(j,n) + \sum_{j<0,n,\gamma} C^+_{j,n,\gamma} J^+(j,n,\gamma)\right. \\
&\qquad \left. + \sum_{j,n} C^{1/2}_{j,n} J^+(j+\frac{1}{2},n) + \sum_{n} C^-_n J^-(n)\right) B .
\end{aligned}
\tag{3.66}
$$

### General method

We now consider the general case for the expansion of

$$
\begin{aligned}
&{}_PF_{P-1}(A_1,...,A_P;B_1,...,B_{P-1},x) = \\
&\quad 1+\frac{\prod_{j=1}^{P-1}\Gamma(B_j)}{\prod_{l=1}^{P}\Gamma(A_l)}\sum_{i=1}^{\infty}\frac{\prod_{l=1}^{P}\Gamma(A_l+i)}{\prod_{j=1}^{P-1}\Gamma(B_j+i)}\frac{x^i}{\Gamma(i+1)} ,
\end{aligned}
\tag{3.67}
$$

with

$$
\begin{aligned}
A_i &= a_i+\frac{1}{2}+\alpha_i\epsilon, \quad 1\leq i\leq r, && A_i = a_i+\alpha_i\epsilon, \quad r<i\leq P \\
B_i &= b_i+\frac{1}{2}+\beta_i\epsilon, \quad 1\leq i\leq s, && B_i = b_i+\beta_i\epsilon, \quad s<i\leq P-1 ,
\end{aligned}
\tag{3.68}
$$

where all $a_i$'s and $b_i$'s are integers. Using the relation

$$x\Gamma(x) = \Gamma(x+1) \qquad \Gamma(x+m) = \Gamma(x+n)\prod_{j}^{n:m}(x+j)\ ,$$

we can transform (3.67) into

$$\begin{aligned}
&{}_PF_{P-1}(a_1+\frac{1}{2}+\alpha_1\epsilon,...,a_P+\alpha_P\epsilon;b_1+\frac{1}{2}+\beta_1\epsilon,...,b_{P-1}+\beta_{P-1}\epsilon,x) = \\
&= 1+\frac{\left(\prod_{l=1}^{s}\Gamma(m_l+\frac{1}{2}+\beta_l\epsilon)\right)\left(\prod_{l=s+1}^{P-1}\Gamma(m_l+\beta_l\epsilon)\right)}{\left(\prod_{l=1}^{r}\Gamma(n_l+1/2+\alpha_l\epsilon)\right)\left(\prod_{l=r+1}^{P}\Gamma(n_l+\alpha_l\epsilon)\right)} \\
&\times \frac{\left(\prod_{l=1}^{s}\prod_{j_l}^{m_l:b_l}(j_l+\frac{1}{2}+\beta_l\epsilon)\right)\left(\prod_{l=s+1}^{P-1}\prod_{j_l}^{m_l:b_l}(j_l+\beta_l\epsilon)\right)}{\left(\prod_{l=1}^{r}\prod_{j_l}^{n_l:a_l}(j_l+\frac{1}{2}+\alpha_l\epsilon)\right)\left(\prod_{l=r+1}^{P}\prod_{j_l}^{n_l:a_l}(j_l+\alpha_l\epsilon)\right)} \\
&\times \sum_{i=1}^{\infty}\underbrace{\frac{\left(\prod_{l=1}^{r}\prod_{j_l}^{n_l:a_l}(i+j_l+\frac{1}{2}+\alpha_l\epsilon)\right)\left(\prod_{l=r+1}^{P}\prod_{j_l}^{n_l:a_l}(i+j_l+\alpha_l\epsilon)\right)}{\left(\prod_{l=1}^{s}\prod_{j_l}^{m_l:b_l}(i+j_l+\frac{1}{2}+\beta_1\epsilon)\right)\left(\prod_{l=s+1}^{P-1}\prod_{j_l}^{m_l:b_l}(i+j_l+\beta_l\epsilon)\right)}}_{D} \\
&\times \frac{\left(\prod_{l=1}^{r}\Gamma(i+n_l+\frac{1}{2}+\alpha_l\epsilon)\right)\left(\prod_{l=r+1}^{P}\Gamma(i+n_l+\alpha_l\epsilon)\right)}{\left(\prod_{l=1}^{s}\Gamma(i+m_l+\frac{1}{2}+\beta_l\epsilon)\right)\left(\prod_{l=s+1}^{P-1}\Gamma(i+m_l+\beta_l\epsilon)\right)}\frac{x^i}{\Gamma(i+1)}\ ,
\end{aligned} \tag{3.69}$$

where the integers $n_i$ and $m_i$ can be chosen as appropriate. The factor $D$ can be partial-fractioned into a sum of factors $i^n$, $1/(i+j+\gamma\epsilon)^n$, or $1/(i+1/2+j+\gamma\epsilon)^n$.

$$D = \sum_{n,j\geq 0}\frac{C^{+}_{j,n}}{(i+j)^n}+\sum_{n,\gamma,j<0}\frac{C^{+}_{j,n,\gamma}}{(i+j+\gamma\epsilon)^n}+\sum_{n,j}\frac{C^{1/2}_{j,n}}{(i+\frac{1}{2}+j)^n}+\sum_{n}C^{-}_{n}i^n\ . \tag{3.70}$$

Again, we write the terms in $D$ as integration or differentiation operators acting on the basis function

$$
\begin{aligned}
& B_s^r(\{n_1,...,n_P;m_1,...,m_{P-1}\},\{\alpha_1,...,\alpha_P;\beta_1,...,\beta_{P-1}\}) \\
\equiv \; & \frac{\left(\prod_{l=1}^{s}\Gamma(m_l+\frac{1}{2}+\beta_l\epsilon)\right)\left(\prod_{l=s+1}^{P-1}\Gamma(m_l+\beta_l\epsilon)\right)}{\left(\prod_{l=1}^{r}\Gamma(n_l+1/2+\alpha_l\epsilon)\right)\left(\prod_{l=r+1}^{P}\Gamma(n_l+\alpha_l\epsilon)\right)} \\
\times \; & \sum_{i=1}^{\infty}\frac{\left(\prod_{l=1}^{r}\Gamma(i+n_l+\frac{1}{2}+\alpha_l\epsilon)\right)\left(\prod_{l=r+1}^{P}\Gamma(i+n_l+\alpha_l\epsilon)\right)}{\left(\prod_{l=1}^{s}\Gamma(i+m_l+\frac{1}{2}+\beta_l\epsilon)\right)\left(\prod_{l=s+1}^{P-1}\Gamma(i+m_l+\beta_l\epsilon)\right)}\frac{x^i}{\Gamma(i+1)} \\
= \; & {}_PF_{P-1}\left(N_1,...,N_P;M_1,...,M_{P-1};x\right)-1
\end{aligned}
\tag{3.71}
$$

obtained by combining the first and last line of (3.69). To shorten the notation, we have used

$$
\begin{aligned}
N_i &= n_i+\frac{1}{2}+\alpha_i\epsilon, \quad 1\le i\le r, & N_i &= n_i+\alpha_i\epsilon, \quad r<i\le P\,, \\
M_i &= m_i+\frac{1}{2}+\beta_i\epsilon, \quad 1\le i\le s, & M_i &= m_i+\beta_i\epsilon, \quad s<i\le P-1\,.
\end{aligned}
\tag{3.72}
$$

We see that the function $B$ defined in (3.57) corresponds to $B_1^1(\{0,1;0\},\{\alpha_1,\alpha_2;\beta_1\})$. The final formula reads

$$
\begin{aligned}
& {}_PF_{P-1}\left(A_1,...,A_P;B_1,...,B_{P-1};x\right) \\
= \; & 1+\frac{\left(\prod_{l=1}^{s}\prod_{j_l}^{m_l:b_l}(j_l+\frac{1}{2}+\beta_l\epsilon)\right)\left(\prod_{l=s+1}^{P-1}\prod_{j_l}^{m_l:b_l}(j_l+\beta_l\epsilon)\right)}{\left(\prod_{l=1}^{r}\prod_{j_l}^{n_l:a_l}(j_l+\frac{1}{2}+\alpha_l\epsilon)\right)\left(\prod_{l=r+1}^{P}\prod_{j_l}^{n_l:a_l}(j_l+\alpha_l\epsilon)\right)} \\
\times \; & \left(\sum_{j\ge 0,n}C_{j,n}^{+}J^{+}(j,n)+\sum_{j<0,n,\gamma}C_{j,n,\gamma}^{+}J^{+}(j,n,\gamma)\right. \\
& \left.\qquad +\sum_{j,n}C_{j,n}^{1/2}J^{+}(j+\frac{1}{2},n)+\sum_{n}C_{n}^{-}J^{-}(n)\right) \\
& B_s^r(\{n_1,...,n_P;m_1,...,m_{P-1}\},\{\alpha_1,...,\alpha_P;\beta_1,...,\beta_{P-1}\})\,.
\end{aligned}
\tag{3.73}
$$

This formula relates a hypergeometric function to another one via differentiation and integration operators. It is therefore sufficient for the expansion of any ${}_PF_{P-1}$ of type $P_s^r$ to have

a) the expansion of *one* HF of the type $P_s^r$ (hereafter called the basis HF)

b) a procedure to integrate the expansion of this basis HF

The expansion of the basis HFs is treated in the next section.

### 3.4.3 All-order expansion of the basis functions

The achievable depth of expansion of a hypergeometric function with half-integer parameters depends on the available depth of the expansion of the corresponding basis functions $B$. In this section we describe how to get an expression for these basis function to arbitrary order in the expansion parameter $\epsilon$.

We first set up some notation. We introduce an associative, distributive but non commutative product $\otimes$ between HPLs of the same argument

$$\begin{aligned} H(s_1,...,s_n;x)\otimes H(t_1,...,t_m;x) &\equiv H(s_1,...,s_n,t_1,...,t_m;x) \\ (H(s_{1...n};x)+H(t_{1...m};x))\otimes H(u_{1...l};x) &\equiv H(s_{1...n},u_{1...l};x)+H(t_{1...m},u_{1...l};x) \\ 1\otimes H(t_1,...,t_m;x) &\equiv H(t_1,...,t_m;x)\ . \end{aligned} \tag{3.74}$$

We can define a "division" with respect to this product

$$H(s_1,...,s_j,...,s_n;x)\oslash H(s_j,...,s_n;x) \equiv H(s_1,...,s_{j-1};x)\ , \tag{3.75}$$

if the vector $t_{1...m}$ is not the last part of the vector $s_{1...n}$ we define

$$H(s_{1...n};x)\oslash H(t_{1...m};x) \equiv 0\ . \tag{3.76}$$

The advantage of this notation is that the derivative "factorises"

$$\begin{aligned} \frac{d}{dx}\left(H(s_{1...n};x)\otimes H(t_{1...m};x)\right) &= \left(\frac{d}{dx}H(s_{1...n};x)\right)\otimes H(t_{1...m};x) \\ \frac{d^j}{dx^j}\left(H(s_{1...n};x)\otimes H(t_{1...m};x)\right) &= \left(\frac{d^j}{dx^j}H(s_{1...n};x)\right)\otimes H(t_{1...m};x) \quad j\le n\ , \end{aligned} \tag{3.77}$$

for a $j$-fold derivative applied on a $\otimes$ product whose left HPL has a weight smaller than $j$ we have no factorization, but we have

$$\left(\frac{d^j}{dx^j}\left(H(s_{1...n};x)\otimes H(t_{1...m};x)\right)\right)\oslash H(t_{1...m};x) = \left(\frac{d^j}{dx^j}H(s_{1...n};x)\right)\ . \tag{3.78}$$

**General strategy**

We make the ansatz

$$B = g(x)\left(1+\sum_{j=1}^{\infty}\epsilon^j \sum_{s_1,\dots s_j=+,0,-} c(s_1,...,s_j;x)H_{s_1,...,s_j}\left(f(x)\right)\right) , \tag{3.79}$$

with $f(x)=\sqrt{x}$ for HFs of type $N_i^i$ and $f(x)=\sqrt{x/(x-1)}$ for HFs of type $N_{i+1}^i$. The function $g(x)$ is given by the value of the HF with the expansion parameter $\epsilon$ put to 0. We see that in the ansatz for HFs of the type $N_{i+1}^i$ we will get HPLs of imaginary arguments for real arguments of the HF to expand. The properties of HPLs of complex arguments are described in chapter 2.

The problem reduces to finding the coefficients $c_{s_1,...,s_j;x}$. Some properties can be stated

- the coefficients $c_{s_1,...,s_j;x}$ are homogeneous of order $j$ in the $\alpha_i, \beta_i$, that means that the powers of the different $\alpha$s and $\beta$s sum up to the same power as $\epsilon$.
- They have to be symmetric in the $\alpha$s and $\beta$s corresponding to equal $a$s or $b$s
- Since an HF ${}_{P+1}F_P$ reduces to an HF ${}_PF_{P-1}$ if two of its parameters are equal, we have conditions on the coefficients $c_{s_1,...,s_j;x}$. If one of the $a$s, say $a_i$ is equal to one of the $b$s, say $b_j$, the coefficient $c$ should reduce to the coefficient of the reduced HF when we take the corresponding $\alpha_i$ and $\beta_j$ to be equal.

The hypergeometric function ${}_PF_{P-1}$ satisfies a differential equation $\mathcal{D}$ of order $P$. Inserting the ansatz in the differential equation

$$\mathcal{D}B = 0$$

the left-hand side can also be written as a sum of HPLs with coefficients

$$\sum_{j=0}^{\infty}\epsilon^j \sum_{l} \sum_{s_1,\dots s_l=+,0,-} \mathcal{D}(s_1,...,s_l)H_{s_1,...,s_l}\left(f(x)\right) = 0 \ . \tag{3.80}$$

The differential equation is satisfied if all the coefficients $\mathcal{D}(s_1,...,s_n)$ vanish. We consider the coefficient $\mathcal{D}$ of a given HPL with weight vector $(v_1,...,v_n)$. Since the differential equation is of order $P$, this coefficient will get contributions from the coefficients $c(...)$ of HPLs of weight $n, n+1, ..., n+P$ with weight vectors of the form $(..., v_1, ..., v_n)$. Using the notation (3.74), that is HPLs of the form,

$$H(s_1,...,s_k,f(x)) \otimes H(v_1,...,s_n,f(x)), \qquad 0 \le k \le P.$$

Thus, for the coefficient $\mathcal{D}(v_1, ..., v_n)$ we only need to consider a part of the ansatz $B$, namely

$$\begin{aligned}\tilde{B}(v_1, ..., v_n; x) &= c(v_1, ..., v_n)g(x) \\ &\times \left(1 + \sum_{j=1}^{P} \epsilon^j \sum_{s_1,...s_j} \tilde{c}(s_{1...j}; x)H(s_{1...j}; f(x))\right) \otimes H(v_1, ..., v_n, f(x)) \; ,\end{aligned} \tag{3.81}$$

where we have defined

$$\tilde{c}(s_{1...j}; x) = \frac{c(s_{1...j}, v_1, ..., v_n; x)}{c(v_1, ..., v_n; x)} \; , \tag{3.82}$$

and where the sum over the weights $s_1, ..., s_j$ runs over $+, -, 0$. The coefficient $\mathcal{D}(v_1, ..., v_n; x)$ is now given by

$$\mathcal{D}(v_1, ..., v_n; x) = \left[\left(\mathcal{D}\tilde{B}(v_1, ..., v_n; x)\right) \oslash H(v_1, ..., v_n; x)\right]_{H(...)=0} \; . \tag{3.83}$$

The only dependence of the right hand side on the vector $(v_1, ..., v_n)$ is in the overall factor $c(s_1, ..., s_j; x)$ and implicitly, in the coefficients $\tilde{c}(s_{1...j}; x)$. Our strategy is now to construct coefficients $\tilde{c}(s_{1...j}; x)$ such that the coefficients (3.83) vanish. In the following, we illustrate this strategy for a simple example.

**Simple example**

We consider the HF

$$ {}_2F_1(\frac{1}{2} + \alpha_1\epsilon, 1 + \alpha_2\epsilon; \frac{1}{2} + \beta_1\epsilon; x) \; , \tag{3.84}$$

making the ansatz

$$B = \frac{1}{1-x}\left(1 + \sum_{j=1}^{\infty} \epsilon^j \sum_{s_1,...s_j=+,0,-} c(s_1, ..., s_j; x)H\left(s_1, ..., s_j; \sqrt{x}\right)\right) . \tag{3.85}$$

We have taken $g(x) = (1-x)^{-1}$ since

$$ {}_2F_1(1, \frac{1}{2}; \frac{1}{2}; x) = \frac{1}{1-x} \; . \tag{3.86}$$

Since the expansion of (3.84) has to be real for negative values of $x$, we have to make sure that the coefficient of the HPLs in the expansion (which will have imaginary argument for $x < 0$) forces the expansion to be real. We know (see Chapter 2) that an HPL of imaginary argument is real if it has an even number of "+" weights and imaginary if the number of "+" weights is odd[5]. Therefore we define

$$\tilde{c}(s_1, ..., s_n; x) = \begin{cases} \sqrt{x} c_o(s_1, ..., s_n) & \text{odd number of } + \text{ in } s_1, ..., s_n \\ c_e(s_1, ..., s_n) & \text{even number of } + \text{ in } s_1, ..., s_n \ . \end{cases}$$

We have now for an even number of "+" in $v_1, ..., v_n$

$$\begin{aligned} \tilde{B}(v_1, ..., v_n; x) &= \frac{c_e(v_1, ..., v_n)}{1-x} \\ \times & \Bigg( 1 + \epsilon \left( \sqrt{x} c_e(+) H(+; \sqrt{x}) + c_e(-) H(-; \sqrt{x}) + c_e(0) H(0; \sqrt{x}) \right) \\ + & \epsilon^2 \Bigg( c_e(+,+) H(+,+; \sqrt{x}) + \sqrt{x} c_e(+,-) H(+,-; \sqrt{x}) \\ & + \sqrt{x} c_e(+,0) H(+,0; \sqrt{x}) + \sqrt{x} c_e(0,+) H(0,+; \sqrt{x}) \\ & + c_e(0,-) H(0,-; \sqrt{x}) + c_e(0,0) H(0,0; \sqrt{x}) \\ & + \sqrt{x} c_e(-,+) H(-,+; \sqrt{x}) + c_e(-,-) H(-,-; \sqrt{x}) \\ & + c_e(-,0) H(-,0; \sqrt{x}) \Bigg) \Bigg) \otimes H(v_1, ..., v_n; \sqrt{x}) \ , \end{aligned} \tag{3.87}$$

and

$$\begin{aligned} \tilde{B}(v_1, ..., v_n; x) &= \frac{c_o(v_1, ..., v_n)}{1-x} = \\ \times & \Bigg( \sqrt{x} + \epsilon \left( c_o(+) H(+; \sqrt{x}) + c_o(-) \sqrt{x} H(-; \sqrt{x}) + c_o(0) \sqrt{x} H(0; \sqrt{x}) \right) \\ + & \epsilon^2 \Bigg( c_o(+,+) \sqrt{x} H(+,+; \sqrt{x}) + c_o(+,-) H(+,-; \sqrt{x}) \\ & + c_o(+,0) H(+,0; \sqrt{x}) + c_o(0,+) H(0,+; \sqrt{x}) + c_o(0,-) \sqrt{x} H(0,-; \sqrt{x}) \\ & + c_o(0,0) \sqrt{x} H(0,0; \sqrt{x}) + c_o(-,+) H(-,+; \sqrt{x}) \\ & + c_o(-,-) \sqrt{x} H(-,-; \sqrt{x}) + c_o(-,0) \sqrt{x} H(-,0; \sqrt{x}) \Bigg) \Bigg) \\ \otimes & \ H(v_1, ..., v_n; \sqrt{x}) \ , \end{aligned} \tag{3.88}$$

for an odd number of "+" in $v_1, ..., v_n$. Inserting these expressions in (3.83) and equating the $\epsilon$ coefficient of the left hand side to zero we get conditions on $c_e(+)$,

[5] provided the last element of the weight vector is not 0, which is not relevant here since such HPLs are divergent at $x = 0$ and we are only interested in solutions of the differential equation regular at $x = 0$.

$c_e(-)$, $c_e(0)$, $c_o(+)$ $c_o(-)$ and $c_o(0)$, namely

$$\begin{aligned} c_e(+) &= \alpha_1 - \beta_1 \qquad c_o(+) = \alpha_2 \\ c_e(-) &= \alpha_2 \qquad c_o(-) = \alpha_1 - \beta_1 \\ c_e(0) &= 0 \qquad c_o(0) = -2\beta_1 \ . \end{aligned} \tag{3.89}$$

These results are independent of the vector $v_1, ..., v_n$, we can thus take this result to define a rule to construct the coefficients of the HPLs in our ansatz (3.85)

$$\begin{aligned} & c(+, w_1, ..., w_n) = \\ & \quad c(w_1, ..., w_n) \times \begin{cases} \alpha_2 & \text{odd number of } + \text{ in } \{w_1, ..., w_n\} \\ \alpha_1 - \beta_1 & \text{even number of } + \text{ in } \{w_1, ..., w_n\} \end{cases} \\ & c(0, w_1, ..., w_n) = \\ & \quad c(w_1, ..., w_n) \begin{cases} -2\beta_1 & \text{odd number of } + \text{ in } \{w_1, ..., w_n\} \\ 0 & \text{even number of } + \text{ in } \{w_1, ..., w_n\} \end{cases} \\ & c(-, w_1, ..., w_n) = \\ & \quad c(w_1, ..., w_n) \times \begin{cases} \alpha_1 - \beta_1 & \text{odd number of } + \text{ in } \{w_1, ..., w_n\} \\ \alpha_2 & \text{even number of } + \text{ in } \{w_1, ..., w_n\} \end{cases} . \end{aligned} \tag{3.90}$$

Using these rules we can show that

$$\mathcal{D}(v_1, ..., v_n; x) = 0$$

for all vectors $(v_1, ..., v_n)$. We can ensure that the boundary conditions are respected by setting

$$c(0) = 0 \qquad c(-) = \alpha_1 \qquad c(+) = \alpha_2 - \beta_1 \ . \tag{3.91}$$

The first terms of the expansion of (3.4.3) are then

$$\begin{aligned} & {}_2F_1(\frac{1}{2} + \alpha_1\epsilon, 1 + \alpha_2\epsilon; \frac{1}{2} + \beta_1\epsilon; x) = \\ & \quad \frac{1}{1-x} \Bigg( 1 + \epsilon \left( \sqrt{x}(\alpha_1 - \beta_1) H(+; \sqrt{x}) + \alpha_2 H(-; \sqrt{x}) \right) \\ & \quad + \ \epsilon^2 \Bigg( \alpha_2(\alpha_1 - \beta_1) H(+, +; \sqrt{x}) + \sqrt{x}(\alpha_1 - \beta_1) H(+, -; \sqrt{x}) \\ & \qquad -2\beta_1(\alpha_1 - \beta_1)\sqrt{x} H(0, +; \sqrt{x}) \\ & \qquad +(\alpha_1 - \beta_1)^2 \sqrt{x} H(-, +; \sqrt{x}) + \alpha_2^2 H(-, -; \sqrt{x}) \Bigg) \Bigg) + \mathcal{O}(\epsilon^3) \ . \end{aligned} \tag{3.92}$$

The success of the strategy relies on the following facts

a) The $x$ dependence of the factors $c(...; x)$ must be known and

b) this dependence must be simple enough in order to minimise the $v_1, ..., v_n$ dependence of the $\tilde{c}(s_{1...j}; x)$ in (3.82)

### 3.4.4 Application to ${}_3F_2$

Since the integration and differentiation operators introduced above with appropriate coefficients allow one to go from one HF to another of the same type $P^r_s$, the choice of which HF should be the basis function is arbitrary. In this section, we show the result of the application of the strategy described in the Section 3.4.3 to an ${}_3F_2$.

**HFs of type $3^1_1$**

We consider the function

$$ {}_3F_2(\frac{1}{2} + \alpha_1\epsilon, 1 + \alpha_2\epsilon, 1 + \alpha_3\epsilon; \frac{1}{2} + \beta_1\epsilon, 1 + \beta_2\epsilon; x) \, . $$

The expansion of this function is best written as a function of the parameters

$$ \begin{aligned} s &= \alpha_2 + \alpha_3 - \beta_2 \\ d_1 &= \alpha_2 - \beta_2 \\ d_2 &= \alpha_3 - \beta_2 \\ d_3 &= \alpha_1 - \beta_1. \end{aligned} \tag{3.93} $$

Like in the example in section 3.4.3 we make the ansatz

$$ \begin{aligned} &{}_3F_2(\frac{1}{2} + \alpha_1\epsilon, 1 + \alpha_2\epsilon, 1 + \alpha_3\epsilon; \frac{1}{2} + \beta_1\epsilon, 1 + \beta_2\epsilon; x) = \\ &\quad \frac{1}{1-x}\left(1 + \sum_{j=1}^{\infty} \epsilon^j \sum_{l\in\{+,0,-\}^j} c(l; x) H_l(\sqrt{x})\right) \, . \end{aligned} \tag{3.94} $$

The coefficient functions are found recursively by applying the following rules

$$ c(l; x) = c(l) \times \begin{cases} \sqrt{x}, & \text{odd number of } + \text{ in } l \\ 1 & \text{even number of } + \text{ in } l \end{cases} \tag{3.95} $$

$$ c(+) = s_2, \quad c(0) = 0, \quad c(-) = s \, . \tag{3.96} $$

The prefactor for + weights makes sure that the expansion is real, as adding a "+" in the weight changes a real HPL into an imaginary one.

$$\begin{aligned}
&c(+,w_1,...,w_n) = \\
&\qquad c(w_1,...,w_n)\begin{cases} s & \text{odd number of + in } \{w_1,...,w_n\} \\ d_3 & \text{even number of + in } \{w_1,...,w_n\} \end{cases} \\
&c(0,w_1,...,w_n) = \\
&\qquad c(w_1,...,w_n)\begin{cases} -2\beta_2 & \text{odd number of + in } \{w_1,...,w_n\} \\ -2\beta_1 & \text{even number of + in } \{w_1,...,w_n\} \text{ and } w_1 = 0 \\ \dfrac{2d_1d_2}{s} & \text{even number of + in } \{w_1,...,w_n\} \text{ and } w_1 \neq 0 \end{cases} \\
&c(-,w_1,...,w_n) = \\
&\qquad c(w_1,...,w_n)\begin{cases} d_3 & \text{odd number of + in } \{w_1,...,w_n\} \\ s & \text{even number of + in } \{w_1,...,w_n\} \end{cases} .
\end{aligned} \tag{3.97}$$

The basis function is then found by subtracting unity from the HF.

$$\begin{aligned}
&B_1^1(\{0,1,1;0,1\},\{\alpha_1,\alpha_2,\alpha_3;\beta_1,\beta_2\}) = \\
&\qquad \frac{1}{1-x}\left(x + \sum_{j=1}^{\infty}\epsilon^j \sum_{l\in\{+,0,-\}^j} c(l;x)H_l(\sqrt{x})\right) .
\end{aligned} \tag{3.98}$$

The expansion of the basis function $B_1^1(\alpha_1,\alpha_2,\beta_1)$ is recovered by setting

$$s \to \alpha_2, \quad d_1, d_2 \to 0, \quad d_3 \to \alpha_1 - \beta_1,$$

and that of the basis function $B_0^0(\alpha_1,\alpha_2,\beta_1)$ by setting

$$s \to \alpha_1+\alpha_2-\beta_1, \quad d_1 \to \alpha_1-\beta_1, \quad d_2 \to \alpha_2-\beta_1, \quad d_3 \to 0 .$$

We see that in this limit all HPLs with weight + disappear from the expansion. Since only HPLs with weight 0 and − can be transformed into HPLs of argument $x^2$ (see chapter 2) we expect only such HPLs to be present in the expansion of HFs with only integer parameters, so that we can convert these HPLs of argument $\sqrt{x}$ into HPLs of argument $x$.

### HFs of the type $3_1^0$

We consider the HF ${}_3F_2(\alpha_1\epsilon, 1+\alpha_2\epsilon, 1+\alpha_3\epsilon; \frac{1}{2}+\beta_1\epsilon, 1+\beta_2\epsilon; x)$ and make the ansatz

$$\begin{aligned}
&{}_3F_2(\alpha_1\epsilon, 1+\alpha_2\epsilon, 1+\alpha_3\epsilon; \frac{1}{2}+\beta_1\epsilon, 1+\beta_2\epsilon; x) = \\
&\qquad 1 + \sum_{j=1}^{\infty}\epsilon^j \sum_{l\in\{+,0,-\}^j} c(l;x)H_l\left(\sqrt{\frac{x}{x-1}}\right) .
\end{aligned} \tag{3.99}$$

The coefficient functions are found recursively by applying the following rules

$$c(l;x) = c(l) \times \begin{cases} \sqrt{\frac{x}{x-1}}, & \text{odd number of } + \text{ in } l \\ 1 & \text{even number of } + \text{ in } l \end{cases} \tag{3.100}$$

$$c(+) = -\alpha_3, \quad c(0) = 0, \quad c(-) = 0 \tag{3.101}$$

$$\begin{aligned}
&c(+,w_1,...,w_n) = c(w_1,...,w_n) \\
&\quad\times \begin{cases} s & \text{odd number of } + \text{ in } \{w_1,...,w_n\} \\ \dfrac{d_1d_2 - s(d_3+\beta_1)}{s} & \text{even number of } + \text{ in } \{w_1,...,w_n\} \text{ and } w_1 = + \\ s - d_1 - d_2 - d_3 + \beta_1 & \text{even number of } + \text{ in } \{w_1,...,w_n\} \text{ and } w_1 \neq + \end{cases} \\
&c(0,w_1,...,w_n) = c(w_1,...,w_n) \\
&\quad\times \begin{cases} -2\beta_2 & \text{odd number of } + \text{ in } \{w_1,...,w_n\} \\ \dfrac{2d_1d_2}{s} & \text{even number of } + \text{ in } \{+,w_1,...,w_n\} \text{ and } w_1 = + \\ 2(d_1+d_2-s) & \text{even number of } + \text{ in } \{w_1,...,w_n\} \text{ and } w_1 \neq + \end{cases} \\
&c(-,w_1,...,w_n) = c(w_1,...,w_n) \\
&\quad\times \begin{cases} -s-\alpha_3 & \text{odd number of } + \text{ in } \{w_1,...,w_n\} \\ \dfrac{d_1d_2}{s} & \text{even number of } + \text{ in } \{+,w_1,...,w_n\} \text{ and } w_1 = + \\ d1 + d_2 - s & \text{even number of } + \text{ in } \{w_1,...,w_n\} \text{ and } w_1 \neq + \,, \end{cases}
\end{aligned} \tag{3.102}$$

where we used the definitions of (3.93). The basis function

$$B_1^0(\{0,1;0\},\{\alpha_1,\alpha_2,\alpha_3;\beta_1,\beta_2\})$$

is then simply

$$B_1^0(\{0,1,1;0,1\},\{\alpha_1,\alpha_2,\alpha_3;\beta_1,\beta_2\}) = \sum_{j=1}^{\infty} \epsilon^j \sum_{l\in\{+,0,-\}^j} c(l;x) H_l\left(\sqrt{\frac{x}{x-1}}\right) . \tag{3.103}$$

The expression for $B_1^0(\{0,1;0\},\{\alpha_1,\alpha_2;\beta_1)\}$ is found by setting

$$s \to \alpha_2, \quad d_1 d_2 \to 0$$

in (3.103).

### HFs of type $3^2_2$

We consider the HF ${}_3F_2(\frac{1}{2}+\alpha_1\epsilon, \frac{1}{2}+\alpha_2\epsilon, 1+\alpha_3\epsilon; \frac{1}{2}+\beta_1\epsilon, \frac{1}{2}+\beta_2\epsilon; x)$ and make the ansatz

$$\begin{aligned} &{}_3F_2(\frac{1}{2}+\alpha_1\epsilon, \frac{1}{2}+\alpha_2\epsilon, 1+\alpha_3\epsilon; \frac{1}{2}+\beta_1\epsilon, \frac{1}{2}+\beta_2\epsilon; x) = \\ &\quad \frac{1}{1-x}\left(1 + \sum_{j=1}^{\infty} \epsilon^j \sum_{l\in\{+,0,-\}^j} c(l;x) H_l\left(\sqrt{\frac{x}{x-1}}\right)\right) . \end{aligned} \tag{3.104}$$

The expansion of this function is best written as a function of the parameters

$$
\begin{aligned}
s &= \alpha_1 + \alpha_2 - \beta_1 - \beta_2 \\
s_\beta &= \beta_1 + \beta_2 \\
p_\alpha &= \alpha_1 \alpha_2 \\
p_\beta &= \beta_1 \beta_2 \ .
\end{aligned} \tag{3.105}
$$

The coefficient functions are found recursively by applying the following rules

$$
\begin{aligned}
c(l;x) &\equiv c(l) \times \begin{cases} \sqrt{\frac{x}{x-1}}, & \text{odd number of } + \text{ in } l \\ 1 & \text{even number of } + \text{ in } l \end{cases} \\
c(+) &= s, \quad c(0) = 0, \quad c(-) = 0
\end{aligned} \tag{3.106}
$$

$$
\begin{aligned}
& c(+, w_1, ..., w_n) = \\
& \qquad c(w_1, ..., w_n) \times \begin{cases} \alpha_3 & \text{odd number of } + \text{ in } \{w_1, ..., w_n\} \\ s & \text{even number of } + \text{ in } \{w_1, ..., w_n\} \end{cases} \\
& c(0, w_1, ..., w_n) = \\
& \qquad \begin{cases} -2 s_\beta c(w_1, ..., w_n) - 4 p_\beta c(w_2, ..., w_n) & \text{odd number of } + \text{ in } \{w_1, ..., w_n\} \\ 0 & \text{even number of } + \text{ in } \{+, w_1, ..., w_n\} \end{cases} \\
& c(-, w_1, ..., w_n) = c(w_1, ..., w_n) \\
& \qquad \begin{cases} s & \text{odd number of } + \text{ in } \{w_1, ..., w_n\} \\ \alpha_3 & \text{even number of } + \text{ in } \{+, w_1, ..., w_n\} \ . \end{cases}
\end{aligned} \tag{3.107}
$$

The basis function $B_2^2(\{0, 0, 1; 0, 0\}, \{\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2)\}$ is then simply

$$
\begin{aligned}
& B_2^2(\{0, 0, 1; 0, 0\}, \{\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2\}) = \\
& \qquad \frac{1}{1-x} \left( x + \sum_{j=1}^{\infty} \epsilon^j \sum_{l \in \{+,0,-\}^j} c(l;x) H_l \left( \sqrt{\frac{x}{x-1}} \right) \right) \ .
\end{aligned} \tag{3.108}
$$

The results of (3.90) are recovered by setting one of $\alpha_1$ or $\alpha_2$ equal to one of the $\beta$'s.

### HFs of type $3_2^1$

For the expansion of the basis function $B_2^1(\{0, 0, 1; 0, 0\}, \{\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2\})$ we consider the expansion of the HF

$$
{}_3F_2(\alpha_1 \epsilon, 1 + \alpha_2 \epsilon, \frac{1}{2} + \alpha_3 \epsilon; \frac{1}{2} + \beta_1 \epsilon, \frac{1}{2} + \beta_2 \epsilon; x) \ , \tag{3.109}
$$

for which we found the expansion

$$\begin{aligned}
&{}_3F_2(\alpha_1\epsilon, 1+\alpha_2\epsilon, \frac{1}{2}+\alpha_3\epsilon; \frac{1}{2}+\beta_1\epsilon, \frac{1}{2}+\beta_2\epsilon; x) = \\
&\qquad 1-\alpha_1\epsilon\omega H(+;\omega) \\
&- \quad \alpha_1\epsilon^2\big((-(\alpha_1+\alpha_2)\,\omega H(-,+;\omega)+\alpha_2 H(+,+;\omega) \\
&\qquad\qquad +2(\alpha_3-\beta_1-\beta_2)\,\omega H(0,+;\omega)\big) \\
&+ \quad \alpha_1\epsilon^3\Big(\alpha_1\alpha_2\omega H(+,+,+;\omega)-(\alpha_1+\alpha_2)^2\,\omega H(-,-,+;\omega) \\
&\qquad -4(\alpha_3-\beta_1-\beta_2)^2\,\omega H(0,0,+;\omega)+\alpha_2(\alpha_1+\alpha_2)\,H(+,-,+;\omega) \\
&\qquad +2(\alpha_1+\alpha_2)(\alpha_3-\beta_1-\beta_2)\,\omega H(0,-,+;\omega) \\
&\qquad -2\alpha_2(\alpha_3-\beta_1-\beta_2)\,H(+,0,+;\omega) \\
&\qquad +2(\alpha_1+\alpha_2)(\alpha_3-\beta_1-\beta_2)\,\omega H(-,0,+;\omega)\Big) \\
&+ \quad 4\epsilon^3\alpha_1(\alpha_3-\beta_1)(\alpha_3-\beta_2)\,\omega H\left(\frac{1}{2},\frac{1}{2},+;\omega\right)+\mathcal{O}(\epsilon^4)\,, \qquad (3.110)
\end{aligned}$$

where

$$\omega = \sqrt{\frac{x}{x-1}}\,.$$

In the last term, we have to define new weights for the HPLs:

$$f_{\frac{1}{2}}(t) = \frac{1}{t\sqrt{1-t^2}}\,. \qquad (3.111)$$

The appearance of this new weight shows that the HPLs of weights $+,-,0$ are not sufficient for the construction of the expansion of all HFs with half-integer parameters. This is however not a limitation to the algorithm described above, so long as one can compute the expansion of one HF of this type, and also integrate products of the type

$$\frac{x^j H\left(\dots,\sqrt{\frac{x}{x-1}}\right)}{\left(\sqrt{1-x^2}\right)^k}\,.$$

This kind of integration also occurs in the algorithm for the easier type of HFs.

## 3.5 Conclusion and outlook

In this chapter we have presented an algorithm to expand hypergeometric functions about integer parameters and a new algorithm to expand hypergeometric functions around half-integer parameters.

The algorithm for integer parameters works for all parameters, and for all ${}_PF_{P-1}$. The algorithm for half-integers works in principle for all parameters, but requires as an ingredient the knowledge of

a) The expansion of *one* HF of the same type as the one to be expanded

b) Integration and differentiation routines for the functions occurring in this expansion.

The method is quite general and might be applied to HFs ${}_PF_{P-1}$ of higher or to other types of HFs.

In this chapter we provide explicitly the all-order expansion of the hypergeometric functions

$$\begin{gathered}
{}_3F_2(\frac{1}{2}+\alpha_1\epsilon,\frac{1}{2}+\alpha_2\epsilon,1+\alpha_3\epsilon;\frac{1}{2}+\beta_1\epsilon,\frac{1}{2}+\beta_2\epsilon;x) \\
{}_3F_2(\frac{1}{2}+\alpha_1\epsilon,1+\alpha_2\epsilon,1+\alpha_3\epsilon;\frac{1}{2}+\beta_1\epsilon,1+\beta_2\epsilon;x) \\
{}_3F_2(\alpha_1\epsilon,1+\alpha_2\epsilon,1+\alpha_3\epsilon;\frac{1}{2}+\beta_1\epsilon,1+\beta_2\epsilon;x)\ .
\end{gathered}$$

These expansions yield the expansion of the HF

$$\begin{gathered}
{}_2F_1(\frac{1}{2}+\alpha_1\epsilon,1+\alpha_2\epsilon;\frac{1}{2}+\beta_1\epsilon;x) \\
{}_2F_1(1+\alpha_1\epsilon,1+\alpha_2\epsilon;\frac{1}{2}+\beta_1\epsilon;x)\ .
\end{gathered}$$

by taking the appropriate limits.

The algorithm for integer parameters has been implemented in the Mathematica Package `HypExp` and is documented in section 3.3. The implementation of the algorithm for half-integer parameters is in progress. Along with the implementation of the algorithm, we need the expansion of basis function for as larger a number of types as possible. It has been seen that the HPLs of weights 0,+,− are not sufficient for HFs with half-integer parameters, so the implementation of new HPL weights will be necessary, if one wants to expand all types of hypergeometric functions $P^r_s$.

The current version of the package `HypExp` has been used for various applications, notably to B physics [10, 33], string theory [34, 35] and the calculation of master integrals [7, 36]

# 3.A Useful relations

In this appendix we collect useful relations among logarithms, polylogarithms $\mathrm{Li}_n$, and Nielsen polylogarithms $S_{n,p}$ as well as some additional integrals. As stated earlier in section 3.3.1, the automatic application of these relations is optional and controlled by the value of `$HypExpPolyLogRules`. The relations are based on refs. [28, 29] and hold at least for all $z \in \mathbb{C}\backslash(1,\infty)$.

### 3.A.1 Relations between logarithms and polylogarithms

$$\ln(\frac{z}{z-1}) = \ln(-z) - \ln(1-z) \tag{3.112}$$
$$\ln(\frac{1}{1-z}) = -\ln(1-z) \tag{3.113}$$
$$\ln(\frac{z}{1-z}) = -\ln(1-z) + \ln(z) \tag{3.114}$$

$$\mathrm{Li}_2(1-z) = -\mathrm{Li}_2(z) + \frac{\pi^2}{6} - \ln(z)\ln(1-z) \tag{3.115}$$
$$\mathrm{Li}_2(\frac{z}{z-1}) = -\mathrm{Li}_2(z) - \frac{1}{2}\ln^2(1-z) \tag{3.116}$$
$$\mathrm{Li}_2(\frac{1}{1-z}) = \mathrm{Li}_2(z) - \frac{1}{2}\ln^2(1-z) + \frac{\pi^2}{6} + \ln(1-z)\ln(-z) \tag{3.117}$$
$$\mathrm{Li}_2(\frac{1}{z}) = -\frac{1}{2}\ln^2(-\frac{1}{z}) - \frac{\pi^2}{6} - \mathrm{Li}_2(z) \tag{3.118}$$
$$\mathrm{Li}_2(\frac{z-1}{z}) = \frac{1}{2}\ln^2(-\frac{1}{z}) + \frac{\pi^2}{3} - \ln(\frac{1}{z})\ln(\frac{z-1}{z}) + \mathrm{Li}_2(z) \tag{3.119}$$

$$\begin{aligned}\mathrm{Li}_3(\frac{z}{z-1}) &= -\mathrm{Li}_3(z) - \mathrm{Li}_3(1-z) + \zeta(3) + \frac{\pi^2}{6}\ln(1-z)\\ &\quad -\frac{1}{2}\ln(z)\ln^2(1-z) + \frac{1}{6}\ \log^3(1-z)\end{aligned} \tag{3.120}$$
$$\begin{aligned}\mathrm{Li}_3(\frac{1}{1-z}) &= \frac{1}{6}\ln^3(1-z) - \frac{1}{2}\ln(-z)\ln^2(1-z) + \frac{1}{2}\ln(z)\ln^2(1-z)\\ &\quad -\frac{\pi^2}{3}\ln(1-z) + \mathrm{Li}_3(1-z)\end{aligned} \tag{3.121}$$
$$\mathrm{Li}_3(\frac{1}{z}) = \mathrm{Li}_3(z) - \frac{\pi^2}{6}\ln(-\frac{1}{z}) - \frac{1}{6}\ln^3(-\frac{1}{z}) \tag{3.122}$$
$$\begin{aligned}\mathrm{Li}_3(\frac{z-1}{z}) &= -\mathrm{Li}_3(z) - \mathrm{Li}_3(1-z) + \zeta(3) - \frac{1}{6}\ln^3(\frac{1-z}{z}) - \frac{\pi^2}{6}\ln(\frac{1-z}{z})\\ &\quad +\frac{1}{6}\ln^3(1-z) + \frac{\pi^2}{6}\ln(1-z) - \frac{1}{2}\ln^2(1-z)\ln(z)\end{aligned} \tag{3.123}$$

$$\begin{aligned}\mathrm{Li}_4(\frac{1}{1-z}) &= -\frac{1}{24}\ln^4(1-z) + \frac{1}{6}\ln(-z)\ln^3(1-z) - \frac{1}{6}\ln(z)\ln^3(1-z)\\ &\quad +\frac{\pi^2}{6}\ln^2(1-z) + \frac{\pi^4}{45} - \mathrm{Li}_4(1-z)\end{aligned} \tag{3.124}$$
$$\mathrm{Li}_4(\frac{z-1}{z}) = -\mathrm{Li}_4(\frac{z}{z-1}) - \frac{1}{24}\ln^4(\frac{1-z}{z}) - \frac{\pi^2}{12}\ln^2(\frac{1-z}{z}) - \frac{7\pi^4}{360} \tag{3.125}$$

$$\begin{aligned}
\mathrm{Li}_5(\frac{1}{1-z}) &= \frac{1}{120}\ln^5(1-z) - \frac{1}{24}\ln(-z)\ln^4(1-z) + \frac{1}{24}\ln(z)\ln^4(1-z) \\
&\quad -\frac{\pi^2}{18}\ln^3(1-z) - \frac{\pi^4}{45}\ln(1-z) + \mathrm{Li}_5(1-z) \qquad (3.126)
\end{aligned}$$

$$\begin{aligned}
S_{2,2}(z) &= \frac{1}{24}\ln^4(1-z) - \frac{1}{6}\ln(z)\ln^3(1-z) + \frac{\pi^2}{12}\ln^2(1-z) \\
&\quad -\mathrm{Li}_3(z)\ln(1-z) + \zeta(3)\ln(1-z) - \mathrm{Li}_4(1-z) + \mathrm{Li}_4(z) \\
&\quad +\mathrm{Li}_4(\frac{z}{z-1}) + \frac{\pi^4}{90} \qquad (3.127) \\
S_{2,2}(1-z) &= -\frac{1}{24}\ln^4(1-z) + \frac{1}{6}\ln(z)\ln^3(1-z) - \frac{1}{4}\ln^2(z)\ln^2(1-z) \\
&\quad -\frac{\pi^2}{12}\ln^2(1-z) + \frac{\pi^2}{6}\ln(z)\ln(1-z) - \ln(z)\,\mathrm{Li}_3(1-z) \\
&\quad +\mathrm{Li}_4(1-z) - \mathrm{Li}_4(z) - \mathrm{Li}_4(\frac{z}{z-1}) + \zeta(3)\ln(z) - \frac{\pi^4}{120} \\
&\qquad (3.128)
\end{aligned}$$

$$\begin{aligned}
S_{2,2}(\frac{z}{z-1}) &= \frac{1}{12}\ln^4(1-z) - \frac{1}{3}\ln(z)\ln^3(1-z) + \frac{\pi^2}{12}\ln^2(1-z) - \frac{\pi^4}{90} \\
&\quad -\mathrm{Li}_3(1-z)\ln(1-z) - \mathrm{Li}_3(z)\ln(1-z) \\
&\quad +\mathrm{Li}_4(1-z) + \mathrm{Li}_4(z) + \mathrm{Li}_4(\frac{z}{z-1}) \\
&\qquad (3.129) \\
S_{2,2}(\frac{1}{1-z}) &= \frac{1}{3}\ln(z)\ln^3(1-z) - \frac{1}{6}\ln(-z)\ln^3(1-z) - \frac{\pi^2}{12}\ln^2(1-z) \\
&\quad -\frac{1}{2}\ln(-z)\ln(z)\ln^2(1-z) + \frac{1}{4}\ln^2(-z)\ln^2(1-z) - \mathrm{Li}_4(z) \\
&\quad -\mathrm{Li}_4(1-z) - \mathrm{Li}_4(\frac{z}{z-1}) + \mathrm{Li}_3(1-z)\ln(1-z) \\
&\quad +\frac{\pi^2}{6}\ln(-z)\ln(1-z) + \frac{\pi^4}{72} - \zeta(3)\ln(1-z) \\
&\quad -\ln(-z)\mathrm{Li}_3(1-z) + \zeta(3)\ln(-z) \qquad (3.130)
\end{aligned}$$

$$\begin{aligned}
S_{2,3}(z) &= \frac{1}{8}\ln(z)\ln^4(1-z) - \frac{1}{30}\ln^5(1-z) - \frac{\pi^2}{18}\ln^3(1-z) \\
&\quad +\frac{1}{2}\mathrm{Li}_3(z)\ln^2(1-z) + \left[\mathrm{Li}_4(1-z) - \mathrm{Li}_4(\frac{z}{z-1})\right]\ln(1-z) \\
&\quad -\frac{\zeta(3)}{2}\ln^2(1-z) - \mathrm{Li}_5(z) - \mathrm{Li}_5(1-z) - \mathrm{Li}_5(\frac{z}{z-1}) \\
&\quad +S_{3,2}(z) + \zeta(5) \qquad (3.131)
\end{aligned}$$

$$
\begin{aligned}
S_{2,3}(1-z) &= \frac{1}{24}\ln(z)\ln^4(1-z)-\frac{1}{6}\ln^2(z)\ln^3(1-z)+\frac{1}{6}\ln^3(z)\ln^2(1-z) \\
&+\frac{\pi^2}{12}\ln(z)\ln^2(1-z)-\frac{\pi^2}{12}\ln^2(z)\ln(1-z)-\mathrm{Li}_4(z)\ln(1-z) \\
&+\zeta(3)\ln(z)\ln(1-z)+\frac{\pi^4}{90}\ln(1-z)+\frac{\pi^4}{90}\ln(z)-\frac{\zeta(3)}{2}\ln^2(z) \\
&+\frac{1}{2}\ln^2(z)\,\mathrm{Li}_3(1-z)-\ln(z)\,\mathrm{Li}_4(1-z)+\ln(z)\,\mathrm{Li}_4(z) \\
&+\ln(z)\,\mathrm{Li}_4(\frac{z}{z-1})-S_{3,2}(z)+2\,\zeta(5)-\frac{\pi^2}{6}\,\zeta(3)
\end{aligned}
\tag{3.132}
$$

$$
\begin{aligned}
S_{2,3}(\frac{1}{1-z}) &= -\frac{1}{60}\ln^5(1-z)+\frac{1}{8}\ln(z)\ln^4(1-z)+\frac{1}{12}\ln^2(-z)\ln^3(1-z) \\
&-\frac{1}{3}\ln(-z)\ln(z)\ln^3(1-z)-\frac{\pi^2}{36}\ln^3(1-z)-\frac{\pi^4}{90}\ln(-z) \\
&-\frac{1}{12}\ln^3(-z)\ln^2(1-z)+\frac{\pi^2}{12}\ln(-z)\ln^2(1-z)-\frac{\zeta(3)}{2}\ln^2(-z) \\
&+\frac{1}{4}\ln^2(-z)\ln(z)\ln^2(1-z)-\frac{\pi^2}{12}\ln^2(-z)\ln(1-z) \\
&+\frac{1}{2}\mathrm{Li}_3(1-z)\ln^2(1-z)-\ln(-z)\ln(1-z)\,\mathrm{Li}_3(1-z) \\
&-\mathrm{Li}_4(1-z)\ln(1-z)-\mathrm{Li}_4(\frac{z}{z-1})\ln(1-z)-\frac{\pi^4}{90}\ln(1-z) \\
&+\frac{1}{2}\ln^2(-z)\,\mathrm{Li}_3(1-z)+\ln(-z)\,\mathrm{Li}_4(1-z)+\ln(-z)\,\mathrm{Li}_4(z) \\
&+\ln(-z)\,\mathrm{Li}_4(\frac{z}{z-1})+\mathrm{Li}_5(1-z)-2\,\mathrm{Li}_5(z)-2\,\mathrm{Li}_5(\frac{z}{z-1}) \\
&+S_{3,2}(z)+\zeta(5)-\frac{\pi^2}{6}\,\zeta(3)
\end{aligned}
\tag{3.133}
$$

$$
\begin{aligned}
S_{2,3}(\frac{z}{z-1}) &= \frac{1}{24}\ln^5(1-z)-\frac{1}{6}\ln(z)\ln^4(1-z)+\frac{\pi^2}{18}\ln^3(1-z)+2\,\zeta(5) \\
&-\frac{1}{2}\mathrm{Li}_3(1-z)\ln^2(1-z)-\frac{1}{2}\mathrm{Li}_3(z)\ln^2(1-z)-S_{3,2}(z) \\
&+\frac{\zeta(3)}{2}\ln^2(1-z)+\left[\mathrm{Li}_4(1-z)+\mathrm{Li}_4(\frac{z}{z-1})\right]\ln(1-z) \\
&+\frac{\pi^4}{90}\ln(1-z)-2\,\mathrm{Li}_5(1-z)+\mathrm{Li}_5(z)+\mathrm{Li}_5(\frac{z}{z-1})
\end{aligned}
\tag{3.134}
$$

$$S_{3,2}(1-z) = -\frac{1}{120}\ln^5(1-z)+\frac{1}{24}\ln(z)\ln^4(1-z)-\frac{1}{12}\ln^2(z)\ln^3(1-z) -\frac{\pi^2}{36}\ln^3(1-z)+\frac{\pi^2}{12}\ln(z)\ln^2(1-z)-\mathrm{Li}_4(z)\ln(1-z) +\zeta(3)\ln(z)\ln(1-z)-\frac{\pi^4}{120}\ln(1-z)+\frac{\pi^4}{90}\ln(z) -\ln(z)\mathrm{Li}_4(1-z)+\mathrm{Li}_5(z)+\mathrm{Li}_5(1-z)+\mathrm{Li}_5(\frac{z}{z-1}) -\frac{\pi^2\zeta(3)}{6}+\zeta(5)-S_{3,2}(z) \tag{3.135}$$

$$S_{3,2}(\frac{z}{z-1}) = \frac{1}{60}\ln^5(1-z)-\frac{1}{24}\ln(z)\ln^4(1-z)+\frac{\pi^2}{36}\ln^3(1-z)+\zeta(5) +\frac{\zeta(3)}{2}\ln^2(1-z)+\left[\mathrm{Li}_4(\frac{z}{z-1})-\mathrm{Li}_4(z)\right]\ln(1-z)+2\mathrm{Li}_5(z) +\frac{\pi^4}{90}\ln(1-z)-\mathrm{Li}_5(1-z)+2\,\mathrm{Li}_5(\frac{z}{z-1})-S_{3,2}(z) \tag{3.136}$$

$$S_{3,2}(\frac{1}{1-z}) = \frac{1}{24}\ln(-z)\ln^4(1-z)-\frac{1}{12}\ln(z)\ln^4(1-z) -\frac{1}{12}\ln^2(-z)\ln^3(1-z)+\frac{1}{6}\ln(-z)\ln(z)\ln^3(1-z) +\frac{\pi^2}{36}\ln^3(1-z)-\frac{\pi^2}{12}\ln(-z)\ln^2(1-z)+\frac{\zeta(3)}{2}\ln^2(1-z) -\mathrm{Li}_4(1-z)\ln(1-z)+\mathrm{Li}_4(z)\ln(1-z)-\frac{\pi^2}{6}\zeta(3) -\frac{\pi^4}{72}\ln(1-z)-\frac{\pi^4}{90}\ln(-z)+\ln(-z)\mathrm{Li}_4(1-z)+2\mathrm{Li}_5(1-z) -\mathrm{Li}_5(z)-\mathrm{Li}_5(\frac{z}{z-1})+S_{3,2}(z)-\zeta(3)\ln(-z)\ln(1-z) \tag{3.137}$$

$$S_{3,2}(-1) = \frac{\pi^2}{12}\zeta(3)-\frac{29}{32}\zeta(5) \tag{3.138}$$

There exist also relations between harmonic polylogarithms $H_{m_1,\ldots,m_k}$ of different arguments. These are implemented in the `HPL` package and described in Ref. [30].

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# Chapter 4

# Implementation of the spinor formalism

*This chapter is based on work done with Pierpaolo Mastrolia.*

## 4.1 Introduction

Upcoming collider experiments, where QCD effects will be ubiquitous, demand high accuracy predictions of processes with many external legs, both for testing the Standard Model in different settings and as backgrounds to new physics processes.

Efficient techniques for computing tree amplitudes have been available for several years [1]. One-loop calculations are considerably more involved, and they constitute a "bottleneck" for obtaining new NLO analytic results.

In principle it is straightforward to compute both tree and loop amplitudes by drawing all Feynman diagrams and evaluating them, using standard reduction techniques for the loop integrals that are encountered. In practice this method becomes extremely inefficient and cumbersome as the number of external legs grows. Consequently, intermediate expressions tend to be vastly more complicated than the final results, when the latter are represented in an appropriate way.

The spinor helicity formalism [2–7] for scattering amplitudes has been an invaluable tool in perturbative computation since its development in the 1980's, being responsible for the existence of compact representations of tree and loop amplitudes. Instead of Lorentz inner products of momenta, it relies on a new set of kinematic objects, spinor products, which neatly capture the collinear behavior of these amplitudes.

The recent boost in the progress of evaluating scattering amplitudes is due to the exploitation of qualitative information on their analytic properties which has been quantitatively turned into tools for computing them. In particular, *on-shell recurrence relations* turn a general property of scattering amplitude, the knowledge of the factorization on poles in the intermediate states, into a technique for computing tree-level amplitudes [8–22]. *Unitarity-based methods* turn another general property of field theory, the unitarity of S-matrix, into a tool to compute amplitudes at loop-level [23–42]. The key ingredient in both cases is the analytic continuation of amplitudes to complex spinor variables [43], which enables the use of lower-point amplitudes as (on-shell) building-blocks in compact spinor-representation for reconstructing (on-shell) amplitudes with larger number of legs and/or loops.

Due to their lower complexity, the expressions obtained by spinor-based methods are numerically more stable and contain many fewer (or no) spurious singularities. In addition, their numerical evaluation is by orders of magnitude [42] faster than that of expressions obtained by other methods, which is of advantage as the speed might become a serious issue when more complicated processes are considered.

This Chapter describes the implementation of the spinor products in the computer algebra program `Mathematica`.

## 4.2 Notation

Positive and negative energy solutions of the massless Dirac equation are identical up to normalization conventions. By closely following the definitions of ref. [44], the solutions of definite helicity

$$u_\pm(k) = \tfrac{1}{2}(1 \pm \gamma_5)u(k) \quad \text{and} \quad v_\mp(k) = \tfrac{1}{2}(1 \pm \gamma_5)v(k) \tag{4.1}$$

and their conjugates

$$\overline{u_\pm(k)} = \overline{u(k)}\tfrac{1}{2}(1 \mp \gamma_5) \quad \text{and} \quad \overline{v_\mp(k)} = \overline{v(k)}\tfrac{1}{2}(1 \mp \gamma_5)\ . \tag{4.2}$$

can be chosen to be equal to each other[1]. We define

$$\begin{aligned} u_+(k_i) &= v_-(k_i) &\equiv& \ |k_i^+\rangle \equiv |i\rangle \\ u_-(k_i) &= v_+(k_i) &\equiv& \ |k_i^-\rangle \equiv |i]\ , \end{aligned} \tag{4.3}$$

and for the conjugate spinors

$$\begin{aligned} \overline{u_+(k_i)} &= \overline{v_-(k_i)} &\equiv& \ \langle k_i^+| \equiv [i|, \\ \overline{u_-(k_i)} &= \overline{v_+(k_i)} &\equiv& \ \langle k_i^-| \equiv \langle i|\ , \end{aligned} \tag{4.4}$$

We define the basic spinor products by

$$\langle i\, j\rangle \ \equiv\ \langle k_i^-|k_j^+\rangle \ =\ \overline{u_-(k_i)}u_+(k_j), \tag{4.5}$$

$$[i\, j] \ \equiv\ \langle k_i^+|k_j^-\rangle \ =\ \overline{u_+(k_i)}u_-(k_j). \tag{4.6}$$

[1]Note that for negative energy solutions, the helicity is the negative of the chirality or $\gamma_5$ eigenvalue

The helicity projection implies that products like $[i|j\rangle$ vanish.

For the numerical evaluation of the spinor products, we use the representation

$$\gamma^0 = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} \mathbf{0} & \sigma^i \\ -\sigma^i & \mathbf{0} \end{pmatrix}, \qquad \gamma_5 = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \quad (4.7)$$

of the Dicac $\gamma$ matrices. In this representation, the massless spinors can be chosen as follows,

$$u_+(k) = v_-(k) = \frac{1}{\sqrt{2}} \begin{bmatrix} \sqrt{k^+} \\ \sqrt{k^-}e^{i\varphi_k} \\ \sqrt{k^+} \\ \sqrt{k^-}e^{i\varphi_k} \end{bmatrix}, \quad u_-(k) = v_+(k) = \frac{1}{\sqrt{2}} \begin{bmatrix} \sqrt{k^-}e^{-i\varphi_k} \\ -\sqrt{k^+} \\ -\sqrt{k^-}e^{-i\varphi_k} \\ \sqrt{k^+} \end{bmatrix}, \quad (4.8)$$

where the phase $e^{\pm i\varphi_k}$

$$e^{\pm i\varphi_k} \equiv \frac{k^1 \pm ik^2}{\sqrt{(k^1)^2 + (k^2)^2}} = \frac{k^1 \pm ik^2}{\sqrt{k^+k^-}}, \qquad k^\pm = k^0 \pm k^3. \quad (4.9)$$

Plugging eqs. (4.8) into the definitions of the spinor products, eq. (4.5), we get explicit formulae for the case when both energies are positive,

$$\begin{aligned} \langle i\, j\rangle &= \sqrt{k_i^- k_j^+}e^{i\varphi_{k_i}} - \sqrt{k_i^+ k_j^-}e^{i\varphi_{k_j}} \\ [i\, j] &= -\sqrt{k_i^- k_j^+}e^{-i\varphi_{k_i}} + \sqrt{k_i^+ k_j^-}e^{-i\varphi_{k_j}}\ . \end{aligned} \quad (4.10)$$

The spinor products are, up to a phase, square roots of Lorentz products, in fact they are related to momenta inner product through the identity,

$$\langle i\, j\rangle\, [j\, i] = \langle i^-|j^+\rangle\langle j^+|i^-\rangle = \mathrm{Tr}\big(\tfrac{1}{2}(1-\gamma_5)\, \not{k}_i\, \not{k}_j\big) = 2k_i \cdot k_j = s_{ij}, \quad (4.11)$$

where $s_{ij} = (k_i + k_j)^2 = 2k_i \cdot k_j$.

The spinor products have simple properties under crossing symmetry, as energies become negative [7]. For negative energies, we define the spinor product $\langle i\, j\rangle$ by analytic continuation from the positive energy case, using the same formula, eq. (4.10), but with $k_i$ replaced by $-k_i$ if $k_i^0 < 0$, and similarly for $k_j$; and with an extra multiplicative factor of $i$ for each negative energy particle.

At the level of the solutions $u$ and $v$ of the Dirac equation we have for $k_0 < 0$

$$u_\pm(k) = iu_\pm(-k)\ . \quad (4.12)$$

We also have the useful identities:

Gordon identity:

$$\langle i|\gamma^\mu|i] = [i|\gamma^\mu|i\rangle = 2k_i^\mu, \quad (4.13)$$

projection operator:

$$|i\rangle[i| = \frac{(1+\gamma_5)}{2}\not{k}_i \qquad |i]\langle i| = \frac{1-\gamma_5}{2}\not{k}_i \qquad |i\rangle[i| + |i]\langle i| = \not{k}_i \tag{4.14}$$

antisymmetry:

$$\langle j\,i\rangle = -\langle i\,j\rangle\,, \qquad [j\,i] = -[i\,j]\,, \qquad \langle i\,i\rangle = [i\,i] = 0 \tag{4.15}$$

Schouten identity:

$$\langle i\,j\rangle\langle k\,l\rangle \;=\; \langle i\,k\rangle\langle j\,l\rangle + \langle i\,l\rangle\langle k\,j\rangle\,. \tag{4.16}$$

Spinor re-definition:

$$\begin{aligned} \not{k}|i\rangle &= |k(i)], & \langle i|\not{k} &= -[k(i)|, \\ \not{k}|i] &= |k(i)\rangle, & [i|\not{k} &= -\langle k(i)| \end{aligned} \tag{4.17}$$

### 4.2.1 Momentum generation

In order to perform checks on expressions containing spinor products, it is useful to have numerical values for the spinor products. In this section we describe the way the package `Sp4m` generates $n$ random momenta $p_i$ satisfying

a) the momentum conservation condition

$$p_1 + ... + p_n = 0\ , \tag{4.18}$$

b) the vectors $p$ are onshell

$$p_i^2 = 0\ .$$

In order to have the sum of the energies vanish, we need some of the momenta to have positive and some to have negative energies (say $m$ positive energies and $n-m$ negative). The first step is to generate two sets of three-vectors

$$\vec{x}_i \qquad i = 1, ..., m \qquad \text{and } \vec{y}_j \qquad j = m+1, ..., n$$

such that the sum of the vectors in each set vanishes. Then one constructs the energies from the three-vector

$$x_i^0 = +\sqrt{\vec{x}_i^2}, \qquad y_i^0 = -\sqrt{\vec{y}_i^2} \tag{4.19}$$

the four vectors $x_i$ and $y_j$ are rescaled according to

$$\hat{x} = \lambda_x x, \quad \lambda_x = \left(\sum_i x_i^0\right)^{-1} \quad \text{and} \quad \hat{y} = \lambda_y y, \quad \lambda_y = \left(\sum_j y_j^0\right)^{-1} \tag{4.20}$$

so that the sum

$$\sum_i \hat{x}_i + \sum_j \hat{y}_j = 0$$

vanishes. The set of vectors containing the vectors $x_i$ and $y_j$ fulfill the requirements a) and b), but there is one disturbing feature namely that the vector part of the sum of the $x_i$'s an $y_j$'s separately vanish, which could lead to accidental cancellations. Indeed, we have

$$\sum_i \hat{x}_i = p = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \sum_j \hat{y}_j = -p = \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{4.21}$$

We can avoid this risk by applying a random boost $B$ to all vectors $\hat{x}_i$ and $\hat{y}_j$.

$$\hat{x}_i \to Bx_1 \equiv X_i, \qquad \hat{y}_j \to By_j \equiv Y_j, \qquad p \to Bp \equiv P \; . \tag{4.22}$$

This method of momenta generation might seem cumbersome, but it has one advantage: one can generate partitions of external vectors, each having a non-vanishing total momentum

$$P = \sum_i X_i = -\sum_j Y_j \; ,$$

as for the momentum across the cuts of loop amplitudes.

## 4.3 Mathematica implementation

In the following section we present the Mathematica implementation. Specific information for notebook users are displayed in italic. The examples are displayed as they look in a notebook. Similar output can be obtained in the shell version by using the command `TraditionalForm`.

After installation, the package is loaded by the input

```
<< Spinor`
```

The package should be loaded at the beginning of the Mathematica session.

*During loading, the default output format is changed to* `TraditionalForm`*, since the output looks better in this format. If this is not wanted, the default setting is recovered using*

```
SetOptions[$FrontEnd, CommonDefaultFormatTypes → {"Output" → StandardForm}]
```

*or with the menu commands*
`Cell` → `Default Output Format Type` → `StandardForm`.

### 4.3.1 New functions

The package introduces the following new functions.

#### Spinors

`DeclareSpinor`

The function `DeclareSpinor` can be called with one or a sequence of arguments. It declares its arguments to be spinors. The symbols representing spinors do not have to be declared as spinors using `DeclareSpinor`, but if it is not the case, some properties are not automatically applied. Integer labels for spinor do not have to be declared, for more details, see the section on `Sp`.

```
DeclareSpinor[a, b, c, d, e, f, i, j, k, l, s, t, u]
{a, b, c, d, e, f, i, j, k, l, s, t, u} added to the List of spinors
```

`SpinorQ`

`SpinorQ` tests whether its argument has been declared as a spinor or not, it returns `True` if so, `False` otherwise. It can be used for example in patterns.

```
SpinorQ[a]
MatchQ[b, _?SpinorQ]
True
True
```

`UndeclareSpinor`

The function `UndeclareSpinor` removes its argument from the list of spinors.

`Sp`

Spinors can be labelled by integers `n` using the function `Sp`. The object `Sp[n]` is considered as a spinor. In the spinor products `Spaa`, `Spab`,`Spba` and `Spbb` described below, integer arguments are automatically enclosed into the `Sp` function.

```
Sp[1]
Sp[1] // FullForm
SpinorQ[Sp[1]]
1
Sp[1]
True
```

*In the notebook, the function* `Sp` *is not displayed but only its argument. The function is only visible in the* `FullForm`

### Slashed matrices

`DeclareSMatrix`

The function `DeclareSMatrix` can be called with one or a sequence of arguments. It declares its arguments to be Dirac matrices. The symbols representing Dirac matrices do not have to be declared as Dirac matrices using `DeclareSMatrix`, but if not done so, some properties can not be used. Integer labels for Dirac matrices do not have to be declared, for more details, see section on `Sm`.

```
DeclareSMatrix[P, Q, R, S, T]
{P, Q, R, S, T} added to the List of Dirac matrix
```

`UndeclareSMatrix`

The function `UndeclareSMatrix` removes its argument from the list of the Dirac matrices.

`SMatrixQ`

`SMatrixQ` tests whether its argument has been declared as a Dirac matrix or not, it returns `True` if so, `False` otherwise. It can be used for example in patterns.

```
SMatrixQ[P]
MatchQ[Q, _?SMatrixQ]
True
True
```

`Sm`

Slashed matrices can be labelled by integers using the function `Sm` the same way as with the function `Sp` for spinors. `Sm[n]` is the slashed matrix corresponding to the momentum labelled by 1. In the spinor products `Spaa`, `Spab`, `Spba` and `Spbb` with slashed matrices enclosed, integer arguments are automatically enclosed into the `Sm` function.

```
Sm[1]
Sm[1] // FullForm
SMatrixQ[Sm[1]]
```

1

Sm[1]

True

*In the notebook, the function* `Sm` *is not displayed but only its argument. The function is only visible in the* `FullForm`

## Invariants

`s[i,j]`

The function `s[i,j]` represents the scalar product

$$s_{ij} = (p_i + p_j)^2 = \langle a\, b\rangle\, [b\, a]$$

Since the `s` is symmetric in its arguments, they are automatically sorted.

```
s[a, b]
s[4, 1]
```

$s_{a\,b}$

$s_{1\,4}$

## Spinor products

`Spaa,Spbb,Spab,Spba`

The functions `Spaa[a,...,b]` represents the spinor product $\langle a...b\rangle$,
`Spab[a,...,b]` the spinor product $\langle a...b]$,
`Spba[a,...,b]` the spinor product $[a...b\rangle$ and
`Spbb[a,...,b]` the spinor product $[a...,b]$.

One can insert symbols representing slashed matrices in the spinor products.

If the leftmost and rightmost objects have been defined as spinors or are positive integers (in which case they are automatically put in `Sp`), more properties are available. These properties are also available if the spinor products contain objects defined as Dirac matrices. These properties are listed below.

### -Standard order

The spinor products have a normal order for their arguments, if the rightmost and leftmost elements are spinors, the middle elements are

Dirac matrices and in addition if the spinors are not in standard order, they are brought to the standard order using the identities

$$\begin{aligned} \langle b\, a\rangle &= -\langle a\, b\rangle\,, & [b\, a] &= -[a\, b]\,, \\ \langle b|Q...P|a\rangle &= -\langle a|P...Q|b\rangle\,, & [b|Q...P|a] &= -[a|P...Q|b]\,, \\ [b|P|a\rangle &= \langle a|P|b]\,, & [b|Q...P|a\rangle &= \langle a|P...Q|b]\,. \end{aligned}$$

A special case of these identities is the on-shell condition

$$\langle a\, a\rangle = 0, \qquad [a\, a] = 0$$

```
Spbb[a, a]
Spaa[nospinor, nospinor]
Spaa[b, a]
Spbb[a, P, Q, b]
Spaa[a, b] Spbb[a, b]
```

0

⟨nospinor | nospinor⟩

$-\langle a\,|\,b\rangle$

$-[b\,|\,Q\,|\,P\,|\,a]$

$-\langle a\,|\,b\rangle\,[b\,|\,a]$

The normal ordering of the Spaa and Spbb products are opposite so that the products $\langle a\, b\rangle\, [b\, a]$ are displayed in this usual way.

**-Linearity**

If the outer arguments of Spaa or Spbb have been defined as spinors using DeclareSpinor, then Spaa and Spbb of linear combinations of spinor are expanded.

```
Spaa[a + b, c]
Spaa[2 b, c]
Spab[a + 2 b, P, a + 3 c - d]
```

$\langle a\,|\,c\rangle + \langle b\,|\,c\rangle$

$2\,\langle b\,|\,c\rangle$

$\langle a\,|\,P\,|\,a] + 3\,\langle a\,|\,P\,|\,c] - \langle a\,|\,P\,|\,d] + 2\,\langle b\,|\,P\,|\,a] + 6\,\langle b\,|\,P\,|\,c] - 2\,\langle b\,|\,P\,|\,d]$

The linearity works for integer labels too, but one has to write the Sp function explicitly, since the sum or product of the integers are done before putting the result in the function Sp.

```
Spaa[1 + 2, 2 coeff]
Spaa[coeff Sp[1], 2]
Spaa[Sp[1] + Sp[2], 3]
```

⟨3 | 2 coeff⟩

coeff ⟨1 | 2⟩

$\langle 1\,|\,3\rangle + \langle 2\,|\,3\rangle$

**-Syntax correction**

When the outer elements of the spinor product are declared as spinor and all inner elements as Dirac matrix, and has a wrong number of Dirac matrices, the type of the spinor product is changed automatically, issuing a warning.

```
Spaa[1, Q, 2]
Spab[1, 2]
Spba[1, Q, P, 2]
Spbb[1, Q, 2]
Spaa::wrongNbrDM : Wrong number of Dirac Martices in the <...> product . Automatically changed to <...]
⟨1 | Q | 2]
Spab::wrongNbrDM : Wrong number of Dirac Martices in the <...] product . Automatically changed to <...>
⟨1|2⟩
Spba::wrongNbrDM : Wrong number of Dirac Martices in the [...> product . Automatically changed to [...]
−[2|P|Q|1]
Spbb::wrongNbrDM : Wrong number of Dirac Martices in the [...] product . Automatically changed to <...]
⟨2 | Q | 1]
```

### Spinor manipulations

`ExpandSToSpinors, ConvertSpinorsToS`

The function `ExpandSToSpinors`, `ConvertSpinorsToS` convert invariants `s` to spinor products and reversely.

```
ExpandSToSpinors[s[1, 2] s[2, 3]]
⟨1|2⟩ ⟨2|3⟩ [2|1] [3 2]
ConvertSpinorsToS[%]
s12 s23
```

`Compactify`

The function `Compactify` compactifies the spinor products using the identities

$$...P|a] = ...|Pa\rangle\,, \qquad ...P|a\rangle = ...|Pa]$$
$$\langle a|P... = -\,[Pa|...\,, \qquad [a|P... = -\,\langle Pa|...$$

```
Compactify[Spab[a, P, b]]
Compactify[Spaa[a, P, Q, b]]
Compactify[Spbb[a, P, Q, b]]
Compactify[Spab[a, P, Q, R, b]]
⟨a | P(b)⟩
⟨a | (P.Q)[b]⟩
[(Q.P)[a] | b]
⟨a | (P.Q.R)[b]⟩
```

One can specify a spinor as second argument for `Compactify`, in which case `Compactify` will only compactify spinor products that contain the given spinor so that the specified spinor is left untouched.

```
Compactify[Spab[a, P, b] + Spab[a, P, c], b]
Compactify[Spaa[a, P, Q, b] + Spab[a, P, c], b]
Compactify[Spaa[a, P, Q, b] + Spab[b, P, c], b]
```

$\langle a \mid P \mid c] - [P(a) \mid b]$

$\langle a \mid P \mid c] - \langle b \mid (Q.P)[a]\rangle$

$\langle b \mid P(c)\rangle - \langle b \mid (Q.P)[a]\rangle$

`UnCompact`

The function `UnCompact` uncompactifies the spinor products compactified with `Compactify`.

```
Compactify[Spab[a, P, b]]
UnCompact[%]
Compactify[Spab[a, P, Q, R, b], b]
UnCompact[%]
```

$\langle a \mid P(b)\rangle$

$\langle a \mid P \mid b]$

$-[(R.Q.P)[a] \mid b]$

$\langle a \mid P \mid Q \mid R \mid b]$

One can specify a spinor as second argument for `UnCompact`, in which case `Compactify` will only uncompactify the spinor product where the Dirac matrices are compactified onto the specified spinor.

```
Compactify[Spaa[a, P, Q, b] + Spab[b, P, c], b]
UnCompact[%]
UnCompact[%%, c]
UnCompact[%%%, a]
```

$\langle b \mid P(c)\rangle - \langle b \mid (Q.P)[a]\rangle$

$\langle a \mid P \mid Q \mid b\rangle + \langle b \mid P \mid c]$

$\langle b \mid P \mid c] - \langle b \mid (Q.P)[a]\rangle$

$\langle b \mid P(c)\rangle + \langle a \mid P \mid Q \mid b\rangle$

`Schouten`

The function `Schouten` applies the Schouten identity

$$\langle i\, j\rangle \langle k\, l\rangle = \langle i\, l\rangle \langle k\, j\rangle + \langle i\, k\rangle \langle j\, l\rangle$$

There are three different possibilities to apply the function.

`Schouten[x,i,j,k,l]`

The function with four spinor arguments will search `x` for occurrences of the products $\langle i\, j\rangle \langle k\, l\rangle$ and replace it using the above identity.

```
Spaa[i, j] Spaa[k, l]
Schouten[%, i, j, k, l]
```

$\langle i \mid j\rangle \langle k \mid l\rangle$

$\langle i \mid k\rangle \langle j \mid l\rangle - \langle i \mid l\rangle \langle j \mid k\rangle$

`Schouten[x,i,j,k]`
: The function with three spinor arguments will search for occurrence of the spinor product $\langle i\, j\rangle$ and will try to use the Schouten identity to combine it with the spinor `k`.

```
Spaa[i, j] Spaa[k, l] Spaa[a, b] + Spaa[i, j] Spaa[a, l] Spaa[k, b]
```

$\langle a \mid b\rangle \langle i \mid j\rangle \langle k \mid l\rangle - \langle a \mid l\rangle \langle b \mid k\rangle \langle i \mid j\rangle$

```
Schouten[%, i, j, k]
```

$\langle a \mid l\rangle (\langle b \mid i\rangle \langle j \mid k\rangle - \langle b \mid j\rangle \langle i \mid k\rangle) + \langle a \mid b\rangle (\langle i \mid k\rangle \langle j \mid l\rangle - \langle i \mid l\rangle \langle j \mid k\rangle)$

`Schouten[x,l]`
: The function with one spinor arguments will search for spinor products

$$\frac{\langle l \ldots}{\langle l \ldots \langle l \ldots}$$

and will use the schouten identity to split it into partial fractions. The function also works for spinor products with embedded Dirac matrices.

```
Spaa[l, u] / (Spaa[l, s] Spaa[l, t])
Schouten[%, l]
```

$\frac{\langle l \mid u\rangle}{\langle l \mid s\rangle \langle l \mid t\rangle}$

$\frac{\langle s \mid u\rangle}{\langle l \mid s\rangle \langle s \mid t\rangle} - \frac{\langle t \mid u\rangle}{\langle l \mid t\rangle \langle s \mid t\rangle}$

```
Spaa[l, u] / (Spaa[l, S, T, s] Spaa[l, t])
```

$\frac{\langle l \mid u\rangle}{\langle l \mid t\rangle \langle l \mid S \mid T \mid s\rangle}$

```
Schouten[%, l]
```

$\frac{\langle s \mid T \mid S \mid u\rangle}{\langle l \mid S \mid T \mid s\rangle \langle s \mid T \mid S \mid t\rangle} - \frac{\langle t \mid u\rangle}{\langle l \mid t\rangle \langle s \mid T \mid S \mid t\rangle}$

### `Sp4m` variables

`$Sp4mFunctions`
: The Symbol `$Sp4mFunctions` contains a list of all functions of the package.

```
$Sp4mFunctions
```
{Compactify, ConvertSpinorsToS, Declare4V, DeclareSMatrix, DeclareSpinor, DeclareSpinorMomentum, ExpandSToSpinors, GenMomenta, Num4V, *s*, Schouten, Sm, SMatrixQ, Sp, Spaa, Spab, Spba, Spbb, SpinorQ, UbarSpa, UbarSpb, UnCompact, UnDeclareSMatrix, UnDeclareSpinor, USpa, USpb}

### Numerics

The spinor products have a numerical implementation. The first step to use this numerical implementation is to generate four-momenta for the particles represented by the spinors. For this there are several possibilities:

**DeclareSpinorMomentum**

This function takes two arguments, first the spinor whose momentum should be set, then the four-vector in the form of a list $\{E, p1, p2, p3\}$. It is the responsability of the user to make sure that the vector indeed is an on-shell vector.

```
DeclareSpinorMomentum[a, {√14, 1, 2, 3}]
DeclareSpinorMomentum[b, {√11, 1, 1, 3}]
DeclareSpinorMomentum[c, {3, 2, 1, -2}]
```
Momentum for spinor *a* set to $\{\sqrt{14}, 1, 2, 3\}$.

Momentum for spinor *b* set to $\{\sqrt{11}, 1, 1, 3\}$.

Momentum for spinor *c* set to $\{3, 2, 1, -2\}$.

Once this is done, the explicit values of the spinors are accessible with the functions `USpa`,`USpb`,`UbarSpa` and `UbarSpa`

```
USpa[c]
USpb[c]
UbarSpa[c]
UbarSpb[c]
```
$$\left\{\frac{1}{\sqrt{2}}, \frac{2+i}{\sqrt{2}}, \frac{1}{\sqrt{2}}, \frac{2+i}{\sqrt{2}}\right\}$$
$$\left\{\frac{2-i}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, -\frac{2-i}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}$$
$$\left\{\frac{2+i}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, \frac{2+i}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right\}$$
$$\left\{\frac{1}{\sqrt{2}}, \frac{2-i}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, -\frac{2-i}{\sqrt{2}}\right\}$$

and one can evaluate spinor products numerically.

```
Spaa[a, b] // N
Spbb[a, b] // N
```
$-0.0651323 + 0.902832\, i$

$0.0651323 + 0.902832\, i$

The values of the momentum associated to the spinor $a$ is accessible through the function `Num4V`

```
Num4V[a]
```

$\{\sqrt{14}, 1, 2, 3\}$

### Declare4V

One can also define four vectors without associated spinors with the function `Declare4V`. It takes two arguments, first the symbol for the vector to be defined and second the value of the four vector in the form of a list. The value stored for the vector can be accessed like for spinor momenta with the function `Num4V`

```
Declare4V[p, {1, 0, 0, 0}]
Num4V[p]
```

Four Momentum $p$ set to {1, 0, 0, 0}.

{1, 0, 0, 0}

Once the four vector is defined, one can use it in spinor products with slashed matrices.

```
Spab[a, p, b] // N
```

$6.9854 + 0.153241\,i$

### GenMomentum

The function `GenMomentum[{s1,...,sn}]` generates arbitrary on-shell four momenta for the spinors `s1,...,sn`, see section 4.2.1. There are generate so that they sum up to 0.

```
GenMomenta[{1, 2, 3, 4, d, e}]
```

Momenta for the spinors 1, 2, 3, 4, $d$, $e$ generated.

Once the momenta are genarated, the (arbitrary but consistent) spinor products and the scalar products can be evaluated.

```
Spaa[1, e] // N
```

$-0.790907 - 1.24331\,i$

```
Spbb[d, 3] // N
```

$-1.03025 + 0.675113\,i$

```
s[1, e] // N
Spaa[1, e] Spbb[e, 1] // N // Chop
```

$-2.17136$

$-2.17136$

The vectors defined for spinor products can also be used as slashed matrices.

```
Spab[1, 3, 2] // N
Spaa[1, 3, 4, 2] // N
```

$0.500852 - 0.291358\,i$

$0.256966 + 0.348538\,i$

## 4.4 Conclusion and outlook

Our goal with `Sp4m`, is to provide the user with a tool for performing basic spinor algebra, plus spinor shifts and the evaluation of residues of spinor variables, needed for a very efficient analytic evaluation of scattering amplitudes at tree- and loop-level, accompanied by the numerical support at every computational stage.

Most of this tasks have been completed yet. The missing parts are the complex shifts of the spinor variables and the reading off of the spinor residues. At the time of writing up this thesis, the package was still in development. More features might be added and details of the implementation might change.

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# Chapter 5

# NLO Antennae for Initial State Radiation

*This chapter is based on the paper*

*"Antenna subtraction with hadronic initial-states" [1]*

*submitted to JHEP with Alejandro Daleo and Thomas Gehrmann.*

## 5.1 Introduction

The calculation of perturbative higher-order corrections to exclusive observables (especially jet production cross sections, but also transverse momentum or rapidity distributions) requires a systematic procedure to extract infrared singularities from real radiation contributions. These singularities arise if one or more final-state particles become soft or collinear. For the task of next-to-leading order (NLO) calculations [2] several systematic and process-independent procedures are available. Except for the phase space slicing technique [3, 4], all these methods [5–10] work by introducing subtraction terms, which are subtracted from the real-radiation matrix element at each phase-space point. These subtraction terms approximate the matrix element in all singular limits, and are sufficiently simple to be integrated over part of the phase-space analytically. After this integration, infrared divergences of the subtraction terms are made explicit, and the integrated subtraction terms can be added to the virtual corrections, thus yielding an infrared-finite result. One of these subtraction methods is antenna subtraction [7–9], which constructs the subtraction terms from so-called antenna functions. These antenna functions describe all unresolved partonic radiation (soft and collinear) between a hard pair of radiator partons.

Extensions to next-to-next-to-leading order (NNLO) are discussed in the literature for phase-space slicing [11], and for several subtraction methods [12–18, 18, 19, 19, 20]. A completely independent approach, avoiding the need for analytical integration is the sector decomposition method, which has been derived for virtual [21, 22] and real radiation [23–26] corrections to NNLO, and applied to several observables already [27–31]. Among the subtraction methods, only the NNLO formulation of the antenna subtraction method [20] has been worked out to a sufficient extent to be readily implemented in the calculation of NNLO corrections to a physical process. Using this method, the calculation of $e^+e^- \to 3$ jets at NNLO accuracy is currently under way [32, 33]. However, up to now, the antenna subtraction (both at NLO and NNLO) method was developed only to handle unresolved singular radiation off final-state partons. An extension to radiation off initial-state partons has been missing so far for this method, while all other NLO subtraction methods could handle radiation off initial- and final-state particles.

In this chapter, we extend the antenna subtraction method to include radiation off initial-state partons, so that it can be used in the calculation of higher order corrections to processes at lepton-hadron or hadron-hadron colliders.

## 5.2 Antenna subtraction

To obtain the perturbative corrections to a jet observable at a given order, all partonic multiplicity channels contributing to that order have to be summed. In general, each partonic channel contains both ultraviolet and infrared (soft and collinear) singularities. The ultraviolet poles are removed by renormalization in each channel. Collinear poles originating from radiation off incoming partons are an inherent feature of the incoming partons, and are cancelled by redefinition (mass factorization) of the parton distributions. The remaining soft and collinear poles cancel among each other only when all partonic channels are summed over.

While infrared singularities from purely virtual corrections are obtained immediately after integration over the loop momenta, their extraction is more involved for real emission (or mixed real-virtual) contributions. Here, the infrared singularities only become explicit after integrating the real radiation matrix elements over the phase space appropriate to the jet observable under consideration. In general, this integration involves the (often iterative) definition of the jet observable, such that an analytic integration is not feasible (and also not appropriate). Instead, one would like to have a flexible method that can be easily adapted to different jet observables or jet definitions. Therefore, the infrared singularities of the real radiation contributions should be extracted using infrared subtraction terms. The crucial points that all subtraction terms must satisfy are that (a) they approximate the full real radiation matrix elements in all singular limits and (b) are still sufficiently simple to be integrated analytically over a section of phase space that encompasses all regions corresponding to singular configurations.

For NLO calculations, several different methods are available to derive subtraction terms in a process-independent way [5–9, 19]. One of these methods is

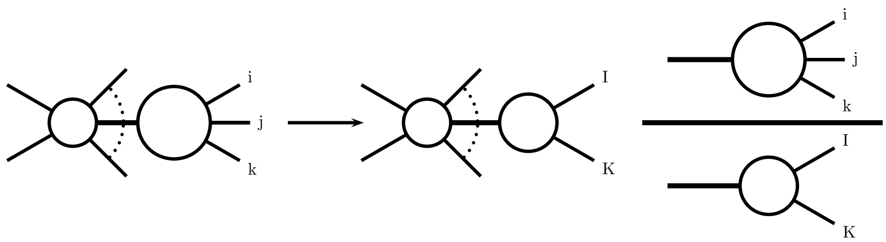


Figure 5.1: Antenna factorization for the final-final situation.

so-called antenna subtraction [7–9].

In this method, antenna functions describe the colour-ordered radiation of unresolved partons between a pair of hard (radiator) partons. All antenna functions at NLO and NNLO can be derived systematically from physical matrix elements, as shown in [20, 34–36]. They can be integrated over the factorized antenna phase space [12] using loop integral reduction techniques extended to phase space integrals [37], and then combined with virtual corrections to partonic processes with lower multiplicity.

Up to now, antenna subtraction has been formulated at NLO [7–9] and NNLO [20] only for processes with a colourless initial-state. In this case, both radiator partons are in the final-state, we call this situation a final-final antenna. For collider observables involving hadronic initial-states, there can be either one or both partons in the initial-state. Unresolved radiation off these initial-state partons can also be subtracted using antenna functions, with one or two radiators in the initial-state. We call these initial-final and initial-initial antennae. The radiated parton is always in the final-state. Figures 5.2–5.2 illustrate how a single unresolved parton can be emitted between radiators in the final or initial-state, and show how all these situations are factorized into antenna functions. Each antenna contains both collinear limits of the unresolved parton with either radiator as well as the soft limit. In each situation, the subtraction term is constructed from products of antenna functions with reduced matrix elements (with fewer final-state partons than the original matrix element), and integrated over a phase space which is factorized into an antenna phase space (involving all unresolved partons and the two radiators) multiplied by a reduced phase space (where the momenta of radiators and unresolved radiation are replaced by two redefined momenta). These redefined momenta can be in the initial-state, if the corresponding radiator momenta were in the initial-state. The full subtraction term is obtained by summing over all antennae required for the problem under consideration. In the most general case (two partons in the initial-state, and two or more hard partons in the final state), this sum includes final-final, initial-final and initial-initial antennae.

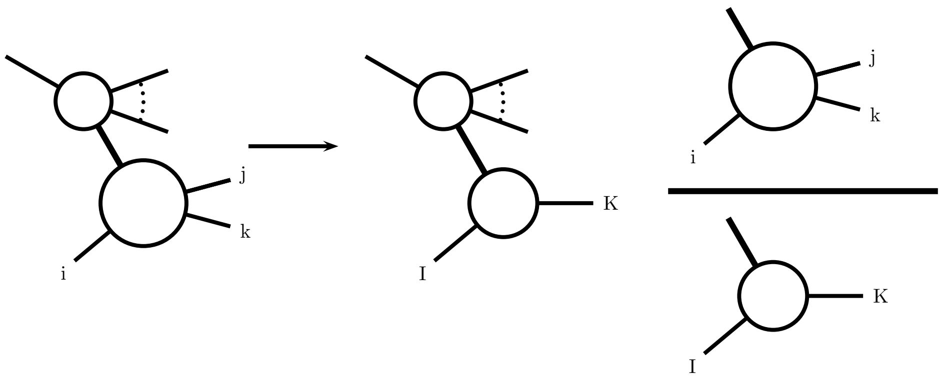


Figure 5.2: Antenna factorization for the initial-final situation.

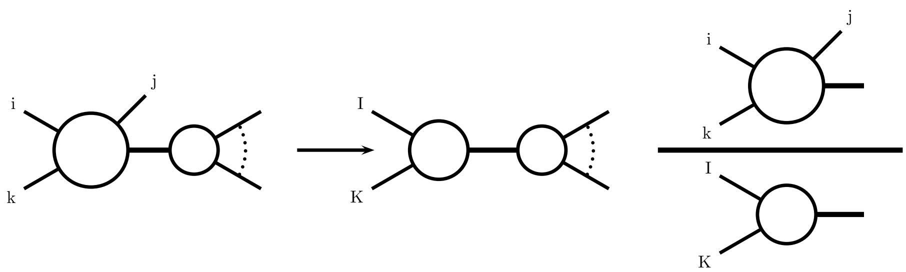


Figure 5.3: Antenna factorization for the initial-initial situation.

To specify the notation, we consider the hadronic cross section

$$\mathrm{d}\sigma = \sum_{a,b} \int \frac{\mathrm{d}\xi_1}{\xi_1}\frac{\mathrm{d}\xi_2}{\xi_2}\, f_{a/1}(\xi_1)\, f_{b/2}(\xi_2)\, \mathrm{d}\hat{\sigma}(\xi_1 H_1, \xi_2 H_2)\ , \tag{5.1}$$

where $\xi_1$ and $\xi_2$ are the momentum fractions of the partons of species $a$ and $b$ in both incoming hadrons, with $f$ being the corresponding parton distribution functions and $H_{1,2}$ denoting the incoming hadron momenta. The cases of only one or no incoming hadrons are obtained trivially by replacing the relevant $f(\xi)$ by $\delta(1-\xi)$. The dependence of the parton-level cross section $\mathrm{d}\hat{\sigma}$ on the parton species $a, b$ is obvious, and not stated explicitly for ease of notation. It should be noted that the parton level cross section $\mathrm{d}\hat{\sigma}$ is normalized to the hadron-hadron flux factor, which is transformed into the parton-parton flux factor by dividing out $\xi_1$ and $\xi_2$ in the above.

We define the partonic tree-level $n$-parton contribution to the $m$-jet cross section (for tree-level cross sections $n = m$; we leave $n \neq m$ for later reference) in $d$ dimensions by,

$$\begin{aligned}\mathrm{d}\hat{\sigma}(p_1,p_2) \quad &= \quad \mathcal{N} \sum_n \mathrm{d}\Phi_n(k_1,\ldots,k_n;p_1,p_2) \\ &\quad\times \frac{1}{S_n}\,|\mathcal{M}_n(k_1,\ldots,k_n;p_1,p_2)|^2\; J_m^{(n)}(k_1,\ldots,k_n).\end{aligned} \tag{5.2}$$

The definition of the observable $J_m^{(n)}(k_1,\ldots,k_n)$ can depend on $H_{1,2}$ (for example through cuts on the jet rapidities), although this is not stated explicitly here. The normalization factor $\mathcal{N}$ includes all QCD-independent factors as well as the dependence on the renormalized QCD coupling constant $\alpha_s$, $\sum_n$ denotes the sum over all configurations with $n$ partons, $\mathrm{d}\Phi_n$ is the phase space for an $n$-parton final-state with total four-momentum $p_1^\mu + p_2^\mu$ in $d = 4-2\epsilon$ space-time dimensions,

$$\begin{aligned}&\mathrm{d}\Phi_n(k_1,...,k_n;p_1,p_2) = \\ &\qquad \frac{\mathrm{d}^{d-1}k_1}{2E_1(2\pi)^{d-1}} \cdots \frac{\mathrm{d}^{d-1}k_n}{2E_n(2\pi)^{d-1}}\,(2\pi)^d\,\delta^d(p_1+p_2-k_1-...-k_n)\,,\end{aligned} \tag{5.3}$$

while $S_n$ is a symmetry factor for identical partons in the final-state. $|\mathcal{M}_n|^2$ denotes a squared, colour-ordered tree-level $n$-parton matrix element.

Antenna subtraction terms $\mathrm{d}\sigma^S$ are constructed using parton-level antenna subtraction terms $\mathrm{d}\hat{\sigma}^S$ as in (5.1), such that

$$\mathrm{d}\sigma - \mathrm{d}\sigma^S$$

is finite in all unresolved limits, and that phase space integrals contained in it can be carried out numerically.

In the following sections, we will briefly summarize the features of antenna subtraction in the final-final case, and derive the antenna phase spaces and antenna functions for the two other cases.

## 5.3 Final-final configurations

In configurations involving final-final antennae, both radiators are in the final-state. This case was described previously in detail at NLO [7–9] and NNLO [20]. The NLO subtraction term for an unresolved parton $j$, emitted between hard final-state radiators $i$ and $k$ is depicted in Figure 5.2. It reads

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^{S,(ff)}(p_1,p_2) = &\mathcal{N}\sum_{m+1}\mathrm{d}\Phi_{m+1}(k_1,\ldots,k_{m+1};p_1,p_2)\frac{1}{S_{m+1}} \\
\times &\sum_{j} X^0_{ijk}\,|\mathcal{M}_m(k_1,\ldots,K_I,K_K,\ldots,k_{m+1};p_1,p_2)|^2 \\
\times &\, J_m^{(m)}(k_1,\ldots,K_I,K_K,\ldots,k_{m+1})
\end{aligned} \tag{5.4}$$

The subtraction term involves the $m$-parton amplitude depending only on the redefined on-shell momenta $k_1,\ldots,K_I,K_K,\ldots,k_{m+1}$ where $K_I,K_K$ are linear combinations of $k_i,k_j,k_k$ while the tree antenna function $X^0_{ijk}$ depends only on $k_i,k_j,k_k$. $X^0_{ijk}$ describes all of the configurations (for this colour-ordered amplitude) where parton $j$ is unresolved.

The jet function $J_m^{(m)}$ in (5.4) does not depend on the individual momenta $k_i$, $k_j$ and $k_k$, but only on $K_I,K_K$. One can therefore carry out the integration over the unresolved dipole phase space appropriate to $k_i$, $k_j$ and $k_k$ analytically, exploiting the factorization of the phase space,

$$\begin{aligned}
&\mathrm{d}\Phi_{m+1}(k_1,\ldots,k_{m+1};p_1,p_2) = \\
&\quad \mathrm{d}\Phi_m(k_1,...,K_I,K_K,...,k_{m+1};p_1,p_2)\cdot \mathrm{d}\Phi_{X_{ijk}}(k_i,k_j,k_k;K_I+K_K,0)\ .
\end{aligned} \tag{5.5}$$

The NLO antenna phase space $\mathrm{d}\Phi_{X_{ijk}}$ is proportional to the three-particle phase space relevant to a $1\to 3$ decay.

At NNLO, one has to consider the emission of one parton in a one-loop corrected process, or the emission of two partons at tree level. Both these were described in detail in ref. [20]. While the one-loop antenna subtraction is largely an extension of the above with the replacement of the tree-level antenna function by a one-loop antenna function, $X^0 \to X^1$, several new features appear in the subtraction of two unresolved partons at tree-level.

In particular, one must pay attention to the colour-connection of the two unresolved partons. If they are colour-unconnected or almost colour-unconnected (sharing a common radiator), the subtraction term is obtained by iterating the procedure employed at NLO, now yielding products of two antenna functions. If both unresolved partons $j,k$ are colour-connected, new four-parton antenna functions $X_{ijkl}$ appear in the subtraction terms:

$$\mathcal{N}\sum_{m+2}\mathrm{d}\Phi_{m+2}(k_1,\ldots,k_{m+2};p_1,p_2)\frac{1}{S_{m+2}}\sum_{jk}\,X^0_{ijkl}$$
$$\times\quad|\mathcal{M}_m(k_1,\ldots,K_I,K_L,\ldots,k_{m+2};p_1,p_2)|^2\,J_m^{(m)}(k_1,\ldots,K_I,K_L,\ldots,k_{m+2})\ ,$$

where the sum runs over all colour-adjacent pairs $j,k$ and implies the appropriate selection of hard momenta $i,l$. As before, the subtraction term involves the $m$-parton amplitude evaluated with on-shell momenta $k_1,\ldots,K_I,K_L,\ldots,k_{m+2}$ where now $K_I$ and $K_L$ are a linear combination of $k_i$, $k_j$, $k_k$ and $k_l$. As for the NLO antenna of the previous section, the tree antenna function $X^0_{ijkl}$ depends only on $k_i,k_j,k_k,k_l$. Particles $i$ and $l$ play the role of the radiators while $j$ and $k$ are the radiated partons.

Once again, the jet function $J_m^{(m)}$ in the above equation depends only on the parent momenta $K_I,K_L$ and not $k_i,\ldots,k_l$. One can therefore carry out the integration over the unresolved antenna phase space (or part thereof) analytically, exploiting the factorization of the phase space,

$$\begin{aligned}&\mathrm{d}\Phi_{m+2}(k_1,\ldots,k_{m+2};p_1,p_2)=\\&\qquad\mathrm{d}\Phi_m(k_1,\ldots,K_I,K_L,\ldots,k_{m+1};p_1,p_2)\cdot\mathrm{d}\Phi_{X_{ijkl}}(k_i,k_j,k_k,k_l;K_I+K_L,0)\ .\end{aligned}\tag{5.6}$$

This phase space factorization must be carried out such that all unresolved limits are reproduced correctly. The most general parameterization for this case is derived in ref. [12]. It should be noted that $\mathrm{d}\Phi_{X_{ijkl}}$ is proportional to the $1\to4$ parton phase space; the analytical integration of the antenna functions over this phase space can thus be carried out with standard methods [37, 38].

## 5.4 Initial-final configurations

In the presence of hadrons in the initial-state, matrix elements exhibit singularities that are not accounted for by the subtraction terms discussed in the previous section. These singularities are due to soft or collinear radiation within an antenna where one or the two hard partons are in the initial-state.

As discussed in ref. [20], the terms necessary to subtract singularities associated with colored particles in the initial-state can be simply obtained by crossing the corresponding antennae for final-state singularities. Due to the different kinematics involved, the factorization of phase space is slightly more involved and the corresponding phase space mappings are different. To cancel explicit infrared poles in virtual contributions and in terms arising from parton distribution mass factorization, the crossed antennae must be integrated, analytically, over the corresponding phase space. In this section we will present the antennae and phase space mappings to subtract singularities when only one of the radiating partons is in the initial-state.

### 5.4.1 Subtraction terms for initial-final singularities

Subtraction terms in the case of one hard parton in the initial-state are built in the same fashion as for the final-final case (formula (2.5) in [20]). We have the following subtraction term associated to a hard radiator parton $i$ with momentum $p$ in the initial-state:

$$\begin{aligned}
&\mathrm{d}\hat{\sigma}^{S,(if)}(p,r) = \mathcal{N} \sum_{m+1} \mathrm{d}\Phi_{m+1}(k_1,\ldots,k_{m+1};p,r)\,\frac{1}{S_{m+1}} \\
&\times \sum_j X^0_{i,jk}\,|\mathcal{M}_m(k_1,\ldots,K_K,\ldots,k_{m+1};xp,r)|^2 \; J^{(m)}_m(k_1,\ldots,K_K,\ldots,k_{m+1})\,.
\end{aligned} \tag{5.7}$$

The additional momentum $r$ stands for the momentum of the second incoming particle, for example, a virtual boson in DIS, or a second incoming parton in a hadronic collision process. This contribution has to be appropriately convoluted with the parton distribution function $f_i$. The tree antenna $X^0_{i,jk}$, depending only on the original momenta $p$, $k_j$ and $k_k$, contains all the configurations in which parton $j$ becomes unresolved. The $m$-parton amplitude depends only on redefined on-shell momenta $k_1,\ldots,K_K,\ldots$, and on the momentum fraction $x$. In the case where the second incoming particle is a parton, there is an additional convolution with the parton distribution of parton $r$ and corresponding subtraction terms associated with it.

The jet function, $J^{(m)}_m$, in (5.7) depends on the momenta $k_j$ and $k_k$ only through $K_K$. Thus, provided a suitable factorization of the phase space, one can perform the integration of the antennae analytically. Due to the hard particle in the initial-state, the factorization of phase space is not as straightforward as for final-final antennae. We start from the $(m+1)$-particle phase space

$$\mathrm{d}\Phi_{m+1}(k_1,\ldots,k_{m+1};p,r) = (2\pi)^d\delta\left(r+p-\sum_l k_l\right)\prod_l [\mathrm{d}k_l] \tag{5.8}$$

where $[\mathrm{d}k] = \mathrm{d}^dk\,\delta(k^2)\Theta(k^0)/(2\pi)^{d-1}$. We insert

$$1 = \int \mathrm{d}^dq\,\delta\left(q+p-k_j-k_k\right)\,, \tag{5.9}$$

and

$$1 = \frac{Q^2}{2\pi}\int\frac{\mathrm{d}x}{x}\int[\mathrm{d}K_K]\,(2\pi)^d\delta\left(q+xp-K_K\right)\,, \tag{5.10}$$

with $Q^2 = -q^2$. Finally, integrating over $q$, the phase space can be factorized in an $m$-parton phase space convoluted with a two particle phase space:

$$\begin{aligned}
\mathrm{d}\Phi_{m+1}(k_1,\ldots,k_{m+1};p,r) &= \mathrm{d}\Phi_m(k_1,\ldots,K_K,\ldots,k_{m+1};xp,r) \\
&\times \frac{Q^2}{2\pi}\mathrm{d}\Phi_2(k_j,k_k;p,q)\frac{\mathrm{d}x}{x}\,.
\end{aligned} \tag{5.11}$$

Replacing the phase space in (5.7), we can explicitly carry out the integration of the antenna factors over the two particle phase space. When combining the integrated subtraction terms with virtual contributions and mass factorization terms, it turns out to be convenient to normalize the integrated antennae as follows

$$\mathcal{X}_{i,jk} = \frac{1}{C(\epsilon)} \int \mathrm{d}\Phi_2 \frac{Q^2}{2\pi} X_{i,jk} \,, \tag{5.12}$$

where

$$C(\epsilon) = (4\pi)^\epsilon \, \frac{e^{-\epsilon\gamma_E}}{8\pi^2} \,. \tag{5.13}$$

The integrated form of the subtraction term is then

$$\begin{aligned}
&\mathrm{d}\hat{\sigma}^{S,(if)}(p,r) = \\
&\quad \sum_{m+1} \sum_j \frac{\mathcal{N}}{S_{m+1}} \int \frac{dx}{x} \, C(\epsilon)\, \mathcal{X}_{i,jk}(x)\, \mathrm{d}\Phi_m(k_1,\ldots,K_K,\ldots,k_{m+1}; x\,p, r) \\
&\quad \times |\mathcal{M}_m(k_1,\ldots,K_K,\ldots,k_{m+1}; x\,p, r)|^2 \\
&\quad \times J_m^{(m)}(k_1,\ldots,K_K,\ldots,k_{m+1}) \,.
\end{aligned} \tag{5.14}$$

Finally, the subtraction term has to be convoluted with the parton distribution functions to give the corresponding contribution to the hadronic cross section. The explicit poles in the integrated form cancel the corresponding ones in the virtual and PDF mass-factorization contributions. To carry out the explicit cancellation of poles, it is convenient to recast, by a simple change of variables, the integrated subtraction term, once convoluted with the PDFs, in the following form

$$\begin{aligned}
d\sigma^{S,(if)}(p,r) \;=\; & \sum_{m+1} \sum_j \frac{S_m}{S_{m+1}} \int \frac{\mathrm{d}\xi_1}{\xi_1} \int \frac{\mathrm{d}\xi_2}{\xi_2} \int_{\xi_1}^1 \frac{\mathrm{d}x}{x} f_{i/1}\left(\frac{\xi_1}{x}\right) \, f_{b/2}\,(\xi_2) \\
& \times C(\epsilon)\, \mathcal{X}_{i,jk}(x)\, \mathrm{d}\hat{\sigma}^B(\xi_1 H_1, \xi_2 H_2) \,.
\end{aligned} \tag{5.15}$$

This convolution has already the appropriate structure and mass factorization can be carried out explicitly leaving a finite contribution. The remaining phase space integration, implicit in the Born cross section, $\mathrm{d}\hat{\sigma}^B$, and the convolutions can be safely done numerically. When considering reactions with only one incoming hadron, the second PDF has to be replaced by a Dirac delta. Reactions with two hadrons will require additional subtractions containing initial-final antennae involving the second parton in the initial-state and initial-initial antennae as well. This case will be discussed in Section 5.5 below.

### 5.4.2 Phase-space mapping

The proper subtraction of infrared singularities requires that the momentum mapping satisfy

$$\begin{array}{llll} xp \to p & K_K \to k_k & \text{when } j \text{ becomes soft} & \\ xp \to p & K_K \to k_j + k_k & \text{when } j \text{ becomes collinear with } k & (5.16) \\ xp \to p - k_j & K_K \to k_k & \text{when } j \text{ becomes collinear with } i & \end{array}$$

In this way, infrared singularities are subtracted locally, except for angular correlations, *before convoluting with the parton distributions.* That is, matrix elements and subtraction terms are convoluted together with PDFs. In addition, the redefined momentum, $K_K$, must be on shell and momentum must be conserved, $p - k_j - k_k = xp - K_K$, for the phase space to factorize as above.

As discussed, in the case of configurations with two hard radiators in the final-state, the three-to-two-parton map of ref. [12] is suitable, as it treats both collinear limits symmetrically and there is only one mapping describing all the singular configurations contained in the antennae.

When subtracting initial-state singularities, however, the mapping of ref. [12] leads to a non factorizing phase space. The decisive point is that this mapping, modified to account for a particle in the initial-state, introduces a new initial-state momentum, $P$ as a linear combination of $p$, $k_j$ and $k_k$. However, as there is no integration over $P$, the factorization of phase space would not be complete, because the $m$-parton matrix elements depend on $P$. On the other hand, if $P$ is proportional to $p$, factorization is granted, in the form of a convolution between the reduced matrix elements and the integrated antennae, as we detailed above. In this case, we immediately obtain the dipole momentum mappings of ref. [5], combined into a single mapping interpolating between all singular limits of the antennae. Explicitly:

$$\begin{aligned} x &= \frac{s_{1j} + s_{1k} - s_{jk}}{s_{1j} + s_{1k}}, \\ K_K &= k_j + k_k - (1 - x)p, \end{aligned} \tag{5.17}$$

where $s_{1j} = (p - k_j)^2$, etc. If parton $j$ becomes soft or collinear to parton $k$, $x \to 1$. If parton $j$ becomes collinear with the initial-state parton $i$, $x = 1 - z$ with $z$ the fraction of $p$ carried by $j$.

The mapping in eq. (5.17) is, in addition, easily generalized to deal with more than one parton becoming unresolved. The building blocks for the double real radiation in the initial-final situation are colour-ordered four-parton antenna functions $X_{i,jkl}$, with one radiator parton $i$ (with momentum $p$) in the initial-state, two unresolved partons $j, k$ and one radiator parton $l$ in the final-state. Starting with the generalization of (5.9) to three particles in the final-state, and combining with (5.10) we have the following mapping at NNLO:

$$\begin{aligned} x &= \frac{s_{1j}+s_{1k}+s_{1l}-s_{jk}-s_{jl}-s_{kl}}{s_{1j}+s_{1k}+s_{1l}}\,, \\ K_L &= k_j+k_k+k_l-(1-x)p\,, \end{aligned} \tag{5.18}$$

where $k_j$, $k_k$ and $k_l$ are the three final-state momenta involved in the subtraction term. This mapping can be obtained from the tripole mapping [37, 39] for final-final configurations at NNLO. It satisfies the appropriate limits in all double singular configurations:

1. $j$ and $k$ soft: $x \to 1$, $K_L \to k_l$,
2. $j$ soft and $k_k \parallel k_l$: $x \to 1$, $K_L \to k_k + k_l$,
3. $k_j = zp \parallel p$ and $k_k$ soft: $x \to 1 - z$, $K_L \to k_l$,
4. $k_j = zp \parallel p$ and $k_k \parallel k_l$: $x \to 1 - z$, $K_L \to k_k + k_l$,
5. $k_j \parallel k_k \parallel k_l$: $x \to 1$, $K_L \to k_j + k_k + k_l$,
6. $k_j + k_k = zp \parallel p$: $x \to 1 - z$, $K_L \to k_l$,

where partons $j$ and $k$ can be interchanged in all cases.

The construction of NNLO antenna subtraction terms requires moreover that all single unresolved limits of the four-parton antenna function $X_{i,jkl}$ have to be subtracted, such that the resulting subtraction term is active only in its double unresolved limits. A systematic subtraction of these single unresolved limits by products of two three-parton antenna functions can be performed only if the NNLO phase space mapping turns into an NLO phase space mapping in its single unresolved limits [12].

In the limits where parton $j$ becomes unresolved, we denote the parameters of the reduced NLO phase space mapping (5.17) by $x'$ and $K'_L$. We find for (5.18):

1. $j$ becomes soft:

$$x \to \frac{s_{1k}+s_{1l}-s_{kl}}{s_{1k}+s_{1l}} = x'\,, \qquad K_L \to k_k+k_l-(1-x)p = K'_L\,.$$

2. $k_j \parallel k_k$, $k_j + k_k = K_K$:

$$x \to \frac{s_{1K}+s_{1l}-s_{Kl}}{s_{1K}+s_{1l}} = x'\,, \qquad K_L \to k_K+k_l-(1-x)p = K'_L\,.$$

3. $k_j = zp \parallel p$:

$$x \to \frac{(1-z)(s_{1k}+s_{1l}) - s_{kl}}{s_{1k}+s_{1l}} = (1-z)x' \,,$$
$$K_L \to k_k + k_l - (1-x')(1-z)p = K'_L.$$

It can be seen that in the first two limits, the NLO mapping involves the original incoming momentum $p$, while in the last limit (initial-state collinear emission), it involves the rescaled incoming momentum $(1-z)p$. To subtract all three single unresolved limits of parton $j$ between emitter partons $i$ and $k$ from $X_{i,jkl}$, one needs to subtract from it the product of two three-parton antenna functions $X_{i,jk} \cdot X_{I,Kl}$. The phase space mapping relevant to these terms is the iteration of two NLO phase space mappings. Analytical integration of these terms with this mapping will result in a double convolution of both antenna functions with the reduced matrix element.

Equally, parton $k$ can become unresolved. Expressing the reduced NLO phase space mapping by $x''$ and $K''_L$. We find for (5.18):

1. $k$ becomes soft:

$$x \to \frac{s_{1j}+s_{1l}-s_{jl}}{s_{1j}+s_{1l}} = x'' \,, \qquad K_L \to k_j + k_l - (1-x)p = K''_L \,.$$

2. $k_k \parallel k_j$, $k_j + k_k = K_K$:

$$x \to \frac{s_{1K}+s_{1l}-s_{Kl}}{s_{1K}+s_{1l}} = x'' \,, \qquad K_L \to k_K + k_l - (1-x)p = K''_L \,.$$

3. $k_k \parallel k_l$, $k_l + k_k = K_K$:

$$x \to \frac{s_{1K}+s_{1j}-s_{Kj}}{s_{1K}+s_{1j}} = x'' \,, \qquad K_L \to k_K + k_j - (1-x)p = K''_L \,.$$

In all limits, the reduced NLO mapping involves the original incoming momentum $p$. Consequently, the three single unresolved limits of parton $k$ between emitter partons $j$ and $l$ can be subtracted from $X_{i,jkl}$ by a product of a final-final and an initial-final three-parton antenna function $X_{jkl} \cdot X_{i,JL}$. The phase space mapping relevant to these terms is the product of an NLO final-final phase space mapping with an initial-final mapping. Integration of the final-final antenna phase space yields an constant, not involving an extra convolution, such that these terms appear in the integrated subtraction term only with a single convolution with the reduced matrix element.

### 5.4.3 NLO antenna functions

We now present explicit results for all the antenna functions necessary to subtract infrared singularities associated with one particle in the initial-state. The unintegrated form of all of them can be obtained from the corresponding expressions for the tree level three-particle antennae in ref. [20] by appropriate crossing of particles from the final to the initial-state. In the cases where there are different particles in the final-state, there is more than one possible crossing and, thus, more than one corresponding antenna.

The invariants for antenna $X_{i,jk}$ are defined as $s = (k_j + k_k)^2$, $t = (p - k_j)^2$, $u = (p - k_k)^2$ and $Q^2 = -q^2$, where $q = p - k_j - k_k$. For the integrated antennae we define $x = Q^2/(2\,p \cdot q)$. The colour-ordered splitting kernels are given by

$$
\begin{aligned}
p^{(0)}_{qq}(x) &= \frac{3}{2}\,\delta(1-x) + 2\mathcal{D}_0(x) - 1 - x\,,\\
p^{(0)}_{qg}(x) &= 1 - 2x + 2x^2\,,\\
p^{(0)}_{gq}(x) &= \frac{2}{x} - 2 + x\,,\\
p^{(0)}_{gg}(x) &= \frac{11}{6}\,\delta(1-x) + 2\mathcal{D}_0(x) + \frac{2}{x} - 4 + 2x - 2x^2\,,\\
p^{(0)}_{gg,F}(x) &= -\frac{1}{3}\,\delta(1-x)\,,
\end{aligned}
\tag{5.19}
$$

where we have introduced the distributions

$$
\mathcal{D}_n(x) = \left(\frac{\ln^n(1-x)}{1-x}\right)_+ .
$$

The colour-ordered infrared singularity operators are as in ref. [20]:

$$
\begin{aligned}
\mathbf{I}^{(1)}_{q\bar{q}}(\epsilon, s_{q\bar{q}}) &= -\frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\left[\frac{1}{\epsilon^2} + \frac{3}{2\epsilon}\right]\mathrm{Re}(-s_{q\bar{q}})^{-\epsilon}\,,\\
\mathbf{I}^{(1)}_{qg}(\epsilon, s_{qg}) &= -\frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\left[\frac{1}{\epsilon^2} + \frac{5}{3\epsilon}\right]\mathrm{Re}(-s_{qg})^{-\epsilon}\,,\\
\mathbf{I}^{(1)}_{gg}(\epsilon, s_{gg}) &= -\frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\left[\frac{1}{\epsilon^2} + \frac{11}{6\epsilon}\right]\mathrm{Re}(-s_{gg})^{-\epsilon}\,,\\
\mathbf{I}^{(1)}_{q\bar{q},F}(\epsilon, s_{q\bar{q}}) &= 0\,,\\
\mathbf{I}^{(1)}_{qg,F}(\epsilon, s_{qg}) &= \frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\,\frac{1}{6\epsilon}\,\mathrm{Re}(-s_{qg})^{-\epsilon}\,,\\
\mathbf{I}^{(1)}_{gg,F}(\epsilon, s_{gg}) &= \frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\,\frac{1}{3\epsilon}\,\mathrm{Re}(-s_{gg})^{-\epsilon}\,.
\end{aligned}
\tag{5.20}
$$

Although the antenna functions are obtained by a simple crossing of the antenna functions for the final-final case, there are some important differences in the decomposition of antenna functions into sub-antennae. In the final-final case, antenna functions involving a hard gluon radiating unresolved gluons had to be split into different configurations since any final-state gluon could be identified as the hard radiator. This ambiguity is no longer present if a gluon is crossed into the initial-state, since an initial-state gluon is hard by kinematical constraints. Instead, a different ambiguity appears, since the initial-state gluon can split either into a quark or into a gluon, thus leading to two possible reduced matrix elements. This ambiguity requires decomposition of the relevant gluon-initiated antenna functions into sub-antennae according to criteria completely different from the final-final situation, as will be discussed in Section 5.4.3 below.

**Quark-initiated antennae**

We consider first antennae with a quark in the initial-state. There is one quark-quark antenna, given by

$$A^0_{q,gq} = -\frac{1}{Q^2}\left(\frac{2u}{s} + \frac{2u}{t} + \frac{2u^2}{st} + \frac{t}{s} + \frac{s}{t}\right) + \mathcal{O}(\epsilon)\,. \tag{5.21}$$

Its integral over the phase space (normalized as in eq. (5.12)) gives

$$\begin{aligned}\mathcal{A}^0_{q,gq} &= -2\mathbf{I}^{(1)}_{q\bar{q}}(Q^2)\,\delta(1-x)\\ &+ (Q^2)^{-\epsilon}\left[-\frac{1}{2\epsilon}p^{(0)}_{qq}(x) + \left(\frac{7}{4} - \frac{\pi^2}{6}\right)\delta(1-x) - \frac{3}{4}\mathcal{D}_0(x) + \mathcal{D}_1(x)\right.\\ &\left.-\frac{3-x}{2} - \frac{1+x}{2}\log(1-x) - \frac{1+x^2}{2(1-x)}\log(x) + \mathcal{O}(\epsilon)\right]\,. \end{aligned}\tag{5.22}$$

There are three quark-gluon antennae given by

$$\begin{aligned}D^0_{q,gg} &= \frac{1}{(Q^2)^2}\left(\frac{s^2}{t} + \frac{s^2}{u} + \frac{t^2}{s} + \frac{4t^2}{u} + \frac{4u^2}{s} + \frac{4u^2}{t} + \frac{3st}{u} + \frac{3su}{t}\right.\\ &\left.+\frac{2t^3}{su} + \frac{2u^3}{st} + \frac{6tu}{s} + 6s + 9t + 9u\right) + \mathcal{O}(\epsilon)\,, \end{aligned}\tag{5.23}$$

$$E^0_{q,q'\bar{q}'} = \frac{1}{(Q^2)^2}\left(\frac{t^2}{s} + \frac{u^2}{s} + t + u\right) + \mathcal{O}(\epsilon)\,, \tag{5.24}$$

$$E^0_{q,qq'} = -\frac{1}{(Q^2)^2}\left(\frac{s^2}{t} + \frac{u^2}{t} + s + u\right) + \mathcal{O}(\epsilon)\,. \tag{5.25}$$

When integrated over the factorized phase space, they yield

$$\begin{aligned}
\mathcal{D}^0_{q,gg} &= -4\mathbf{I}^{(1)}_{qg}(Q^2)\delta(1-x) \\
&+ (Q^2)^{-\epsilon}\left[-\frac{1}{\epsilon}p^{(0)}_{qq}(x) + \left(\frac{67}{18} - \frac{1}{3}\pi^2\right)\delta(1-x) - \frac{11}{6}\mathcal{D}_0(x) + 2\mathcal{D}_1(x)\right. \\
&\left. -\frac{1}{3x} + 1 - x - (1+x)\log(1-x) - \frac{1+x^2}{1-x}\log(x) + \mathcal{O}(\epsilon)\right], \qquad (5.26)
\end{aligned}$$

$$\begin{aligned}
\mathcal{E}^0_{q,q'\bar{q}'} &= -4\mathbf{I}^{(1)}_{qg,F}(Q^2)\delta(1-x) \\
&+(Q^2)^{-\epsilon}\left[-\frac{5}{9}\delta(1-x) + \frac{1}{3}\mathcal{D}_1(x) - \frac{1}{6x} + \mathcal{O}(\epsilon)\right], \qquad (5.27)
\end{aligned}$$

$$\mathcal{E}^0_{q,qq'} = (Q^2)^{-\epsilon}\left[-\frac{1}{2\epsilon}p^{(0)}_{gq}(x) + \frac{2}{x} - \frac{3}{2} - \frac{(2-2x+x^2)}{2x}\log\left(\frac{1-x}{x}\right) + \mathcal{O}(\epsilon)\right]. \qquad (5.28)$$

Finally, there is one gluon-gluon antenna with a quark in the initial-state:

$$G^0_{q,qg} = -\frac{1}{(Q^2)^2}\left(\frac{s^2}{t} + \frac{u^2}{t}\right) + \mathcal{O}(\epsilon)\,, \qquad (5.29)$$

yielding

$$\mathcal{G}^0_{q,qg} = (Q^2)^{-\epsilon}\left[-\frac{1}{2\epsilon}p^{(0)}_{gq}(x) - \frac{7}{4x} + 1 + \frac{(2-2x+x^2)}{2x}\log\left(\frac{1-x}{x}\right) + \mathcal{O}(\epsilon)\right], \qquad (5.30)$$

when integrated over the antenna phase space.

### Gluon-initiated antennae

For gluon-initiated antennae, we find one quark-quark antenna

$$A^0_{g,q\bar{q}} = \frac{1}{Q^2}\left(\frac{2s}{t} + \frac{2s}{u} + \frac{2s^2}{tu} + \frac{u}{t} + \frac{t}{u}\right) + \mathcal{O}(\epsilon)\,. \qquad (5.31)$$

Its integrated form is

$$\mathcal{A}^0_{g,q\bar{q}} = (Q^2)^{-\epsilon}\left[-\frac{1}{\epsilon}p^{(0)}_{qg}(x) - (1-2x+2x^2)\left(\log\frac{1-x}{x}\right) + \mathcal{O}(\epsilon)\right]. \qquad (5.32)$$

There is one quark-gluon antenna with a gluon in the initial-state

$$\begin{aligned}
D^0_{g,qg} &= \frac{1}{(Q^2)^2}\left(\frac{u^2}{t} + \frac{u^2}{s} + \frac{4t^2}{s} + \frac{4t^2}{u} + \frac{4s^2}{u} + \frac{4s^2}{t} + \frac{3tu}{s} + \frac{3su}{t}\right. \\
&+ \left.\frac{2t^3}{su} + \frac{2s^3}{tu} + \frac{6st}{u} + 6u + 9t + 9s\right) + \mathcal{O}(\epsilon)\,. \qquad (5.33)
\end{aligned}$$

This antenna is singular when the quark or the gluon in the final-state becomes collinear with the initial-state gluon. In the first case it collapses into a quark-gluon antenna and in the second case into a gluon-quark one. Accordingly, the reduced matrix elements accompanying these two singular configurations are different. Thus, the antenna must be split to separate these two configurations. This can be easily done by partial fractioning in the variables $t$ and $u$, we obtain

$$D^0_{g,qg} = -\frac{1}{2}\frac{1}{(Q^2)^2}\left(\frac{2u^2}{t}+\frac{8s^2}{t}+\frac{6su}{t}-\frac{4s^3}{t(Q^2+s)}\right)+\mathcal{O}(\epsilon)\,, \qquad (5.34)$$

and

$$\begin{aligned} D^0_{g,gq} &= \frac{1}{2}\frac{1}{(Q^2)^2}\left(\frac{2t^2}{s}+\frac{8u^2}{s}+\frac{8u^2}{t}+\frac{8s^2}{t}+\frac{6tu}{s}+\frac{4u^3}{st}-\frac{4s^3}{(Q^2+s)t}\right. \\ &\left. +\frac{12su}{t}+12t+18u+18s\right)+\mathcal{O}(\epsilon)\,, \end{aligned} \qquad (5.35)$$

where we have adjusted the names of the antennae so that $D^0_{g,ij}$ now does not contain singularities when $j$ becomes collinear with the initial-state gluon. We also changed the sign of the first sub-antenna and exchanged $t$ and $u$ in the second case to agree with the definitions given at the beginning of the section. The two sub-antennae can be integrated over the factorized phase space, namely:

$$\begin{aligned} \mathcal{D}^0_{g,qg} &= (Q^2)^{-\epsilon}\left[-\frac{1}{2\,\epsilon}p^{(0)}_{qg}(x)+\frac{3}{4x}-1+\frac{1}{2}(1-2x+2x^2)\log(1-x)\right. \\ &\left. -\frac{1}{2}\,(1-2x+2x^2)\log(x)+\mathcal{O}(\epsilon)\right]\,. \end{aligned} \qquad (5.36)$$

and

$$\begin{aligned} \mathcal{D}^0_{g,gq} &= -2\mathbf{I}^{(1)}_{qg}(Q^2)\delta(1-x)+(Q^2)^{-\epsilon}\left[-\frac{1}{2\epsilon}p^{(0)}_{gg}(x)+\left(\frac{7}{4}-\frac{1}{6}\pi^2\right)\delta(1-x)\right. \\ &-\frac{3}{4}\mathcal{D}_0(x)+\mathcal{D}_1(x)-\frac{3}{2}+\frac{1-2x+x^2-x^3}{x}\log(1-x) \\ &\left.-\frac{(1-x+x^2)^2}{x(1-x)}\log(x)+\mathcal{O}(\epsilon)\right]\,. \end{aligned} \qquad (5.37)$$

Finally there are two gluon-gluon antennae

$$\begin{aligned} F^0_{g,gg} &= \frac{1}{2}\frac{1}{(Q^2)^2}\left(\frac{8s^2}{t}+\frac{8t^2}{s}+\frac{8s^2}{u}+\frac{8u^2}{s}+\frac{8t^2}{u}+\frac{8u^2}{t}+\frac{12st}{u}+\frac{12su}{t}+\frac{12tu}{s}\right. \\ &\left.+\frac{4t^3}{su}+\frac{4u^3}{st}+\frac{4s^3}{tu}+24s+24t+24u\right)+\mathcal{O}(\epsilon)\,, \end{aligned} \qquad (5.38)$$

$$G^0_{g,q\bar{q}} = \frac{1}{(Q^2)^2}\left(\frac{t^2}{s}+\frac{u^2}{s}\right)+\mathcal{O}(\epsilon)\,. \qquad (5.39)$$

Their integrated forms are given by:

$$\begin{aligned}
\mathcal{F}^0_{g,gg} &= -4\mathbf{I}^{(1)}_{gg}(Q^2)\delta(1-x) \\
&+ \quad (Q^2)^{-\epsilon}\left[-\frac{1}{\epsilon}p^{(0)}_{gg}(x)+\left(\frac{67}{18}-\frac{1}{3}\pi^2\right)\delta(1-x)-\frac{11}{6}\mathcal{D}_0(x)\right. \\
&\qquad +2\mathcal{D}_1(x)-\frac{11}{6x}+\frac{2(1-2x+x^2-x^3)}{x}\log(1-x) \\
&\qquad \left.-\frac{2(1-x+x^2)^2}{x(1-x)}\log(x)+\mathcal{O}(\epsilon)\right], \qquad (5.40)\\
\mathcal{G}^0_{g,q\bar{q}} &= -2\mathbf{I}^{(1)}_{gg,F}(Q^2)\delta(1-x) \\
&\quad +(Q^2)^{-\epsilon}\left[-\frac{5}{9}\delta(1-x)+\frac{1}{3}\mathcal{D}_1(x)+\frac{1}{3x}+\mathcal{O}(\epsilon)\right]. \qquad (5.41)
\end{aligned}$$

## 5.5 Initial-initial configurations

The last situation to be considered is when the two hard radiators are in the initial-state. The subtraction terms necessary to account for singularities associated with these configurations are constructed in terms of initial-initial antennae. At NLO, one unresolved parton is emitted off these two radiators, as displayed in Figure 5.2. As before, more final-state partons can be emitted at higher orders.

The initial-initial configuration is slightly more involved than the previous two. Even though at NLO the integration of the antenna functions over the factorized phase space will turn out to be trivial, in order to guarantee this factorization, only a very restricted kind of mapping will be allowed. In addition, to fulfill overall momentum conservation, both the hard radiators and *all* the spectator momenta, including non-colored particles, have to be remapped. This is done with a convenient generalization of the Lorentz transformation introduced in ref. [5].

### 5.5.1 Subtraction terms for initial-initial configurations

The NLO antenna subtraction term, to be convoluted with the appropriate parton distribution functions for the initial-state partons, for a configuration with the two hard emitters in the initial-state (partons $i$ and $k$ with momenta $p_1$ and $p_2$) can be written as:

$$\begin{aligned}
d\hat{\sigma}^{S,(ii)} &= \mathcal{N}\sum_{m+1}\mathrm{d}\Phi_{m+1}(k_1,\ldots,k_{j-1},k_j,k_{j+1},\ldots,k_{m+1};p_1,p_2)\,\frac{1}{S_{m+1}} \\
&\quad \sum_j X^0_{ik,j}(p_1,p_2,k_j)\left|\mathcal{M}_m(\tilde{k}_1,\ldots,\tilde{k}_{j-1},\tilde{k}_{j+1},\ldots,\tilde{k}_{m+1};x_1p_1,x_2p_2)\right|^2 \\
&\quad \times J^{(m)}_m(\tilde{k}_1,\ldots,\tilde{k}_{j-1},\tilde{k}_{j+1},\ldots,\tilde{k}_{m+1}). \qquad (5.42)
\end{aligned}$$

As mentioned, all the momenta in the arguments of the reduced matrix elements and the jet functions have been redefined. The two hard radiators are simply rescaled by factors $x_1$ and $x_2$ respectively. The spectator momenta are boosted by a Lorentz transformation onto the new set of momenta $\{\tilde{k}_l,\, l \neq j\}$. As before, the mapping must satisfy overall momentum conservation and keep the mapped momenta on the mass shell. In this case, this turns out to severely restrict the possible mappings.

We start from the $(m+1)$-parton phase space

$$\mathrm{d}\Phi_{m+1}(k_1,\ldots,k_{m+1};p_1,p_2) = (2\pi)^d\delta\left(p_1+p_2-\sum_l k_l\right)\prod_l[\mathrm{d}k_l] \tag{5.43}$$

and insert

$$1 = \int \mathrm{d}^d q \mathrm{d}^d \tilde{q}\, \delta\left(p_1+p_2-k_j-q\right)\, \delta\left(x_1p_1+x_2p_2-\tilde{q}\right)\,, \tag{5.44}$$

and

$$1 = \int \prod_{l\neq j} \delta(\tilde{k}_l - B(k_l,q,\tilde{q}))[\mathrm{d}\tilde{k}_l]\,, \tag{5.45}$$

where $B$ is a Lorentz transformation that maps $q$ onto $\tilde{q}$. We also insert

$$1 = \int \mathrm{d}x_1\mathrm{d}x_2\delta(x_1-\hat{x}_1)\delta(x_2-\hat{x}_2) \tag{5.46}$$

with

$$\begin{aligned}
\hat{x}_1 &= \left(\frac{s_{12}-s_{j2}}{s_{12}}\,\frac{s_{12}-s_{1j}-s_{j2}}{s_{12}-s_{1j}}\right)^{\frac{1}{2}}\,, \\
\hat{x}_2 &= \left(\frac{s_{12}-s_{1j}}{s_{12}}\,\frac{s_{12}-s_{1j}-s_{j2}}{s_{12}-s_{j2}}\right)^{\frac{1}{2}}\,.
\end{aligned} \tag{5.47}$$

These last two definitions guarantee overall momentum conservation in the mapped momenta and the right soft and collinear behavior, they are derived in detail in Section 5.5.2 below. Now we can integrate over the original momenta, $k_l\,, l \neq j$ by inverting the Lorentz transformation. The Jacobian factor associated with this integration is unity, as $B$ is a proper Lorentz transformation. We also integrate over the auxiliary momenta $q$ and $\tilde{q}$, to obtain

$$\begin{aligned}
\mathrm{d}\Phi_{m+1}(k_1,\ldots,k_{m+1};p_1,p_2) &= \mathrm{d}\Phi_m(\tilde{k}_1,\ldots,\tilde{k}_{j-1},\tilde{k}_{j+1},\ldots,\tilde{k}_{m+1};x_1p_1,x_2p_2) \\
&\quad \times\delta(x_1-\hat{x}_1)\,\delta(x_2-\hat{x}_2)\,[\mathrm{d}k_j]\,\mathrm{d}x_1\,\mathrm{d}x_2\,.
\end{aligned} \tag{5.48}$$

At this point the phase space is totally factorized into the convolution of an $m$ particle phase space, involving only the redefined momenta, with the phase space of parton $j$.

Inserting the factorized expression for the phase space measure in eq. (5.42), the subtraction terms can be integrated over the antenna phase space. The integrated form of the subtraction terms must be, then, combined with the virtual and mass factorization terms to cancel the explicit poles in $\epsilon$. In the case of initial-initial subtraction terms, the antenna phase space is trivial: the two remaining Dirac delta functions can be combined with the one particle phase space, such that there are no integrals left. We define the initial-initial integrated antenna functions as follows:

$$\mathcal{X}_{ik,j}(x_1,x_2) = \frac{1}{C(\epsilon)} \int [\mathrm{d}k_j]\, x_1\, x_2\, \delta(x_1-\hat{x}_1)\, \delta(x_2-\hat{x}_2)\, X_{ik,j} \tag{5.49}$$

Substituting the one particle phase space, and carrying out the integrations over the Dirac delta functions[1], we have,

$$\mathcal{X}_{ik,j}(x_1,x_2) \;=\; (Q^2)^{-\epsilon} \frac{e^{\epsilon\gamma_E}}{\Gamma(1-\epsilon)} \mathcal{J}(x_1,x_2)\, Q^2\, X_{ik,j}\,, \tag{5.50}$$

with $Q^2 = q^2 = (p_1+p_2-k_j)^2$. The Jacobian factor, $\mathcal{J}(x_1,x_2)$ is given by

$$\mathcal{J}(x_1,x_2) = \frac{x_1\, x_2\, (1+x_1\, x_2)}{(x_1+x_2)^2}\, (1-x_1)^{-\epsilon} (1-x_2)^{-\epsilon} \left( \frac{(1+x_1)(1+x_2)}{(x_1+x_2)^2} \right)^{-\epsilon}, \tag{5.51}$$

and the two-particle invariants are given by:

$$s_{1j} = -s_{12} \frac{x_1\,(1-x_2^2)}{x_1+x_2}\,, \qquad s_{j2} = -s_{12} \frac{x_2\,(1-x_1^2)}{x_1+x_2}\,. \tag{5.52}$$

The integrated subtraction term is then,

$$\begin{aligned} \mathrm{d}\hat{\sigma}^{S,(ii)} \;=\;& \sum_{m+1} \sum_j \frac{\mathcal{N}}{S_{m+1}} \int \frac{\mathrm{d}x_1}{x_1} \frac{\mathrm{d}x_2}{x_2}\, C(\epsilon)\, \mathcal{X}_{ik,j}(x_1,x_2) \\ & \times \mathrm{d}\Phi_m(k_1,\ldots,k_{j-1},k_{j+1},\ldots,k_{m+1}; x_1 p_1, x_2 p_2) \\ & \times |\mathcal{M}_m(k_1,\ldots,k_{j_1},k_{j+1},\ldots,k_{m+1}; x_1 p1, x_2 p_2)|^2 \\ & \times J_m^{(m)}(k_1,\ldots,k_{j-1},k_{j+1},\ldots,k_{m+1})\,, \end{aligned} \tag{5.53}$$

where we have relabeled all $\tilde{k}_i \to k_i$. The final step is to convolute this subtraction term with the parton distribution functions of the initial-state particles. The integrated version of the subtraction pieces is then combined with the virtual and mass-factorization terms to yield a finite contribution when $\epsilon \to 0$. Recasting the convolutions appropriately, the integrated subtraction term is

$$\begin{aligned} d\sigma^{S,(ii)} \;=\;& \sum_{m+1} \sum_j \frac{S_m}{S_{m+1}} \int \frac{\mathrm{d}\xi_1}{\xi_1} \int \frac{\mathrm{d}\xi_2}{\xi_2} \int_{\xi_1}^1 \frac{\mathrm{d}x_1}{x_1} \int_{\xi_2}^1 \frac{\mathrm{d}x_2}{x_2} f_{i/1}\left(\frac{\xi_1}{x_2}\right) f_{k/2}\left(\frac{\xi_2}{x_2}\right) \\ & \times C(\epsilon)\, \mathcal{X}_{ik,j}(x_1,x_2)\, \mathrm{d}\hat{\sigma}^B(\xi_1 H_1, \xi_2 H_2)\,. \end{aligned} \tag{5.54}$$

[1]see Appendix 5.B for more details.

### 5.5.2 Phase-space mapping

By asking for momentum conservation and phase-space factorization, we are severely constraining the possible phase-space mappings. The principal origin of this constraint is that the remapping of both initial-state momenta can only be a rescaling, since any transversal component would spoil the phase space factorization.

The two mapped initial-state momenta must be of the form

$$P_1 = x_1 p_1 \qquad P_2 = x_2 p_2 \,, \tag{5.55}$$

so that

$$\tilde{q} \equiv P_1 + P_2$$

is in the beam axis. Since the vector component of $q \equiv p_1 + p_2 - k_j$ is in general not along the $p_1 - p_2$ axis we need to boost all the other momenta in order to restore momentum conservation. The transformation must map $q$ onto $\tilde{q}$. As it must keep all the spectator momenta, which are arbitrary vectors, on the mass shell, it must belong to the Lorentz group. This transformation then fully determines the initial-initial phase-space mapping, by fixing $x_{1,2}$ in terms of the invariants.

We consider a candidate Lorenz transformation $\Lambda(q)$. It has to map the vector $q$ into a vector $\Lambda(q)q = \tilde{q}$ in the beam axis. From the result $\tilde{q}$ of the transformation, one can read off $x_1$ and $x_2$ using

$$\begin{aligned} 2(p_1 + p_2)\tilde{q} &= (x_1 + x_2)s_{12} \\ 2(p_1 - p_2)\tilde{q} &= (x_2 - x_1)s_{12} \end{aligned}$$

yielding

$$\begin{aligned} x_1 &= \frac{2p_2\tilde{q}}{s_{12}} \\ x_2 &= \frac{2p_1\tilde{q}}{s_{12}} \end{aligned} \tag{5.56}$$

The two equations can be combined to give

$$x_1 x_2 = \frac{s_{12} - s_{1j} - s_{2j}}{s_{12}} \,,$$

which can also be derived from the on shell condition $q^2 = \tilde{q}^2$. To ensure that the mapping has the right soft and collinear limits at NLO it is sufficient to impose $\Lambda(q) = 1$ for $q$ in the beam axis.

For the transformation $\Lambda$ we take a boost $B^*_T(q)$ of appropriate parameter whose direction is transverse to the beam axis in the rest frame of $P_1$ and $P_2$. Objects defined in the rest frame of the new system are denoted by a $^*$. This transformation clearly satisfies the requirement $B^*_T(q) = 1$ for $q$ in the beam axis, since then no boost is required to bring $q$ into the beam axis. By construction, the longitudinal component of $q$ in the rest frame of $P_1$ and $P_2$ is conserved, that is

$$q_L^* = \frac{(P_1 - P_2)q}{x_1 x_2 \sqrt{s}} = \tilde{q}_L^* = \frac{(P_1 - P_2)\tilde{q}}{x_1 x_2 \sqrt{s}} . \tag{5.57}$$

So that we have

$$(x_2 - x_1) = \frac{x_2 s_{2j} - x_1 s_{1j}}{s_{12}} \tag{5.58}$$

which gives the mapping

$$\begin{aligned} x_1 &= \sqrt{\frac{s_{12} - s_{2j}}{s_{12} - s_{1j}}} \sqrt{\frac{s_{12} - s_{1j} - s_{2j}}{s_{12}}}, \\ x_2 &= \sqrt{\frac{s_{12} - s_{1j}}{s_{12} - s_{2j}}} \sqrt{\frac{s_{12} - s_{1j} - s_{2j}}{s_{12}}} , \end{aligned} \tag{5.59}$$

which was used in (5.47) above. It yields the correct soft and collinear limits at NLO:

1. $j$ soft: $x_1 \to 1$, $x_2 \to 1$.
2. $k_j = z_1 p_1 \parallel p_1$: $x_1 = (1 - z_1)$, $x_2 = 1$.
3. $k_j = z_2 p_2 \parallel p_2$: $x_1 = 1$, $x_2 = (1 - z_2)$.

It should be pointed out the transformation is not unique. Possible transformations are however strongly constrained. If one requires a symmetrical treatment of $x_1$ and $x_2$, rotations are not allowed as part of the transformation. To show that, we take $p_j$ to be transverse to the beam axis. Bringing $q$ to the beam axis with a rotation will force us to choose to rotate $\vec{q}$ either towards the $p_1$ or the $p_2$ side. This would favor either $x_1$ or $x_2$. The only way to bring $q$ to the beam axis, without having to choose between $x_1$ and $x_2$ is in this case a boost transverse to the beam axis.

The extension of the phase space mapping to NNLO is trivial. In this case, four-parton antenna functions $X_{il,jk}$ require a mapping with two partons, $j$ and $k$ unresolved. The transformation $B_T^*(q)$ is unchanged, but now the vector $q$ is given by $q = p_1 + p_2 - k_j - k_k$. The momentum fractions in (5.47) are replaced by

$$\begin{aligned} x_1 &= \left( \frac{s_{12} - s_{j2} - s_{k2}}{s_{12}} \, \frac{s_{12} - s_{1j} - s_{1k} - s_{j2} - s_{k2} + s_{jk}}{s_{12} - s_{1j} - s_{1k}} \right)^{\frac{1}{2}} , \\ x_2 &= \left( \frac{s_{12} - s_{1j} - s_{1k}}{s_{12}} \, \frac{s_{12} - s_{1j} - s_{1k} - s_{j2} - s_{k2} + s_{jk}}{s_{12} - s_{j2} - s_{k2}} \right)^{\frac{1}{2}} . \end{aligned} \tag{5.60}$$

These two momentum fractions satisfy the following limits in double unresolved configurations:

1. $j$ and $k$ soft: $x_1 \to 1$, $x_2 \to 1$,
2. $j$ soft and $k_k = z_1 p_1 \parallel p_1$: $x_1 \to 1 - z_1$, $x_2 \to 1$,
3. $k_j = z_1 p_1 \parallel p_1$ and $k_k = z_2 p_2 \parallel p_2$: $x_1 \to 1 - z_1$, $x_2 \to 1 - z_2$,
4. $k_j + k_k = z_1 p_1 \parallel p_1$: $x_1 \to 1 - z_1$, $x_2 \to 1$,

and all the limits obtained from the ones above by exchange of $p_1$ with $p_2$ and of $k_j$ with $k_k$. The factorization of the phase space into an $m$-parton phase space and an antenna phase space goes along the same lines as for the NLO case. At NNLO, however, the integration of the antenna functions over this factorized phase space is no longer trivial.

As in the initial-final case, we also require the NNLO mapping to turn into the NLO mapping (5.47) if only one parton becomes unresolved. In the limits where $j$ becomes unresolved between $i$ and $k$, we denote the parameters of the reduced NLO phase space mapping by $x_1'$ and $x_2'$. We find:

1. $j$ becomes soft:

$$
\begin{aligned}
x_1 &\to \left(\frac{s_{12}-s_{k2}}{s_{12}}\,\frac{s_{12}-s_{1k}-s_{k2}}{s_{12}-s_{1k}}\right)^{\frac{1}{2}} = x_1'\,, \\
x_2 &\to \left(\frac{s_{12}-s_{1k}}{s_{12}}\,\frac{s_{12}-s_{1k}-s_{k2}}{s_{12}-s_{k2}}\right)^{\frac{1}{2}} = x_2'
\end{aligned}
$$

2. $k_j \parallel k_k$, $k_j + k_k = K_K$:

$$
\begin{aligned}
x_1 &\to \left(\frac{s_{12}-s_{K2}}{s_{12}}\,\frac{s_{12}-s_{1K}-s_{K2}}{s_{12}-s_{1K}}\right)^{\frac{1}{2}} = x_1'\,, \\
x_2 &\to \left(\frac{s_{12}-s_{1K}}{s_{12}}\,\frac{s_{12}-s_{1K}-s_{K2}}{s_{12}-s_{K2}}\right)^{\frac{1}{2}} = x_2'\,.
\end{aligned}
$$

3. $k_j = z_1 p_1 \parallel p_1$:

$$
\begin{aligned}
x_1 &\to \left(\frac{(1-z_1)s_{12}-s_{k2}}{s_{12}}\,\frac{(1-z_1)s_{12}-(1-z_1)s_{1k}-s_{k2}}{s_{12}-s_{1k}}\right)^{\frac{1}{2}} = (1-z_1)x_1'\,, \\
x_2 &\to \left(\frac{s_{12}-s_{1k}}{s_{12}}\,\frac{(1-z_1)s_{12}-(1-z_1)s_{1k}-s_{k2}}{(1-z_1)s_{12}-s_{k2}}\right)^{\frac{1}{2}} = x_2'\,.
\end{aligned}
$$

All other single unresolved limits involving one radiator parton in the initial-state follow by exchange of $p_1$ with $p_2$ or $k_j$ with $k_k$. To subtract all unresolved limits of parton $j$ between emitter partons $i$ and $k$ from $X_{il,jk}$, one needs to subtract from it the product of an initial-final antenna function with an initial-initial antenna function $X_{i,jk} \cdot X_{Il,K}$. Analytic integration of these terms over both antenna phase spaces results in a double convolution in the rescaling variables for $p_1$ and a single convolution in the rescaling variable for $p_2$.

At subleading colour, $j$ can also become unresolved between $i$ and $l$. In this case, we denote the reduced phase space mapping parameters by $x_1''$ and $x_2''$. The limits read:

1. $j$ becomes soft:

$$
\begin{aligned}
x_1 &\rightarrow \left(\frac{s_{12}-s_{k2}}{s_{12}}\,\frac{s_{12}-s_{1k}-s_{k2}}{s_{12}-s_{1k}}\right)^{\frac{1}{2}} = x_1''\,,\\
x_2 &\rightarrow \left(\frac{s_{12}-s_{1k}}{s_{12}}\,\frac{s_{12}-s_{1k}-s_{k2}}{s_{12}-s_{k2}}\right)^{\frac{1}{2}} = x_2''
\end{aligned}
$$

2. $k_j = z_1 p_1 \parallel p_1$:

$$
\begin{aligned}
x_1 &\rightarrow \left(\frac{(1-z_1)s_{12}-s_{k2}}{s_{12}}\,\frac{(1-z_1)s_{12}-(1-z_1)s_{1k}-s_{k2}}{s_{12}-s_{1k}}\right)^{\frac{1}{2}} = (1-z_1)x_1''\,,\\
x_2 &\rightarrow \left(\frac{s_{12}-s_{1k}}{s_{12}}\,\frac{(1-z_1)s_{12}-(1-z_1)s_{1k}-s_{k2}}{(1-z_1)s_{12}-s_{k2}}\right)^{\frac{1}{2}} = x_2''\,.
\end{aligned}
$$

3. $k_j = z_2 p_2 \parallel p_2$:

$$
\begin{aligned}
x_1 &\rightarrow \left(\frac{s_{12}-s_{k2}}{s_{12}}\,\frac{(1-z_2)s_{12}-s_{1k}-(1-z_2)s_{k2}}{(1-z_2)s_{12}-s_{1k}}\right)^{\frac{1}{2}} = x_1''\,,\\
x_2 &\rightarrow \left(\frac{(1-z_2)s_{12}-s_{1k}}{s_{12}}\,\frac{(1-z_2)s_{12}-s_{1k}-(1-z_2)s_{k2}}{s_{12}-s_{k2}}\right)^{\frac{1}{2}} = (1-z_2)x_2''\,.
\end{aligned}
$$

These single unresolved limits are subtracted from $X_{il,jk}$ by the product of two initial-initial antenna functions $X_{il,j} \cdot X_{IL,k}$. Analytic integration of these terms over both antenna phase spaces results in two double convolutions in the rescaling variables for $p_1$ and $p_2$.

### 5.5.3 NLO antenna functions

The unintegrated antenna functions necessary to subtract all the singular configurations at NLO with two initial-state hard radiators, can be obtained immediately from the corresponding initial-final ones quoted in section 5.4.3 by crossing. We have

$$X^0_{ik,j} = \delta_{ik,j}\, X^0_{j,ik}\,, \tag{5.61}$$

where $\delta_{ik,j}$ is an overall sign, which is $-1$ for $D^0_{gg,q}$ and $E^0_{q\bar{q},q'}$ and $+1$ for all other antennae.

The Mandelstam variables of the unintegrated antennae in section 5.4.3 have to be replaced by $s = (p_i + p_k)^2$, $t = (p_i - p_j)^2$, $u = (p_k - p_j)^2$.

Again, the splitting of antenna functions into different sub-antennae is different from the two configurations discussed above. For the initial-initial configurations there is no need to split the quark-gluon antenna $D^0_{qg,g}$ as in all the singular limits it collapses to the same two-particle antenna. So $D^0_{qg,g}$ is given by the crossing of (5.33). However, in this case, the antenna $D^0_{gg,q}$ has to be split into two subantennae to separate the two collinear limits present in it. We find:

$$D^0_{gg,q} = D^0_{g_1 g_2,q} + D^0_{g_2 g_1,q}\,, \tag{5.62}$$

such that $D^0_{g_1 g_2,q}$ contains only the singular configurations when the quark becomes collinear with gluon $g_2$. Explicitly:

$$D^0_{g_1 g_2,q} = \frac{1}{(Q^2)^2}\left(\frac{s^2}{u} + \frac{4t^2}{u} + \frac{4u^2}{s} + \frac{3st}{u} + \frac{2t^3}{su} + \frac{3tu}{s} + 3s + 9u\right) + \mathcal{O}(\epsilon)\,, \tag{5.63}$$

As mentioned, the integration of the initial-initial antennae over the factorized phase space is trivial and only involves a proper treatment of the singularities when $\epsilon \to 0$. The integrated antennae read

$$
\begin{aligned}
\mathcal{A}^0_{qg,q} &= (Q^2)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{qg}(x_2)\,\delta(1-x_1) \\
&+\left(\frac{1}{2}+\frac{1-2x_2+2x_2^2}{2}\log\left(2\frac{1-x_2}{1+x_2}\right)\right)\delta(1-x_1) \\
&+\mathcal{D}_0(x_1)\frac{1-2x_2+2x_2^2}{2}-\frac{1-2x_2+2x_2^2}{2(1-x_1)} \\
&+\frac{x_1(1+x_1x_2)\left(2x_1x_2^3+x_2^2+\left(2x_2^4-2x_2^2+1\right)x_1^2\right)}{(x_1+x_2)^3\left(1-x_1^2\right)} \\
&+\frac{x_1x_2(1+x_1x_2)\left(2x_1-x_2\left(x_1^2+2x_2x_1-1\right)\right)}{(x_1+x_2)^3}\Bigg], \qquad (5.64)\\
\mathcal{A}^0_{q\bar{q},g} &= -\mathbf{I}^{(1)}_{q\bar{q}}(Q^2)\delta(1-x_1)\delta(1-x_2)+(Q^2)^{-\epsilon}\left[-\frac{1}{2\epsilon}p^{(0)}_{qq}(x_1)\delta(1-x_2)\right] \\
&+(Q^2)^{-\epsilon}\Bigg[\frac{\left(x_1^2+x_2^2\right)\left(x_2^2x_1^2+2x_2x_1^2+x_1^2+3x_2x_1+2x_1+1\right)}{2(x_1+1)(x_2+1)(x_1+x_2)^2} \\
&+\frac{\left((1-x_1)^2-2x_1^2\log\left(\frac{1+x_1}{2}\right)+\left(1-x_1^2\right)\log\left(\frac{2}{1-x_1^2}\right)\right)\delta(1-x_2)}{2(1-x_1)} \\
&+\frac{1}{4}\pi^2\delta(1-x_1)\delta(1-x_2)-\frac{1}{2}(1+x_2)\mathcal{D}_0(x_1)+\frac{1}{2}\mathcal{D}_0(x_1)\mathcal{D}_0(x_2) \\
&+\delta(1-x_1)\mathcal{D}_1(x_2)+(x_1\leftrightarrow x_2)\Bigg], \qquad (5.65)\\
\mathcal{D}^0_{qg,g} &= -2\left(\mathbf{I}^{(1)}_{qg}(Q^2)\right)\delta(1-x_1)\delta(1-x_2) \\
&+(Q^2)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{qq}(x_1)\delta(1-x_2)-\frac{1}{2\epsilon}p^{(0)}_{gg}(x_2)\delta(1-x_1) \\
&+\frac{\pi^2}{2}\delta(1-x_1)\delta(1-x_2)+\delta(1-x_2)\mathcal{D}_1(x_1)+\delta(1-x_1)\mathcal{D}_1(x_2) \\
&+\left(\frac{1-x_1}{2}+\frac{\log\left(\frac{2}{x_1+1}\right)}{1-x_1}-\frac{1+x_1}{2}\log\left(2\frac{1-x_1}{x_1+1}\right)\right)\delta(1-x_2) \\
&+\left(-x_2^2+x_2-2+\frac{1}{x_2}\right)\mathcal{D}_0(x_1)-\frac{1+x_1}{2}\mathcal{D}_0(x_2)+\mathcal{D}_0(x_1)\mathcal{D}_0(x_2) \\
&+\frac{(x_1x_2-1)\left(x_2^2x_1^4+\left(2x_2^3+x_2\right)x_1^3+\left(2x_2^4-x_2^2+4\right)x_1^2\right)(x_1x_2+1)^2}{x_1\left(1-x_1^2\right)(x_1+x_2)^3\left(1-x_2^2\right)} \\
&+\frac{(x_1x_2-1)\left(5x_1x_2+2x_2^2\right)(x_1x_2+1)^2}{x_1\left(1-x_1^2\right)(x_1+x_2)^3\left(1-x_2^2\right)} \\
&+\frac{x_2^2-x_2+2-\frac{1}{x_2}}{1-x_1}+\frac{4-x_1x_2\left(x_2+x_1\left(x_1^2+x_1+1\right)(x_2+1)-3\right)}{2x_1x_2\left(1-x_1^2\right)\left(1-x_2^2\right)} \\
&+\left(\frac{\log\left(\frac{2}{x_2+1}\right)}{1-x_2}-\frac{\left(x_2^3-x_2^2+2x_2-1\right)\log\left(2\frac{1-x_2}{x_2+1}\right)}{x_2}\right)\delta(1-x_1)\Bigg], \qquad (5.66)
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{D}^0_{g_1 g_2,q} &= (Q^2)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{qg}(x_2)\delta(1-x_1) \\
&\quad +(Q^2)^{-\epsilon}\left(\frac{1}{2}+\frac{1-2x_2+2x_2^2}{2}\log\left(2\frac{1-x_2}{1+x_2}\right)\right)\delta(1-x_1) \\
&\quad +\frac{\left(2x_2x_1^3+x_1^2+x_2^2\left(2x_1^4-2x_1^2+1\right)\right)\left(1+x_2x_1\right)^2}{\left(1-x_2^2\right)\left(x_2+x_1\right)^4} \\
&\quad -\frac{\left(4x_1^2x_2^4+3\left(2x_1^3+x_1\right)x_2^3\right)\left(x_2x_1+1\right)}{2(x_2+x_1)^4} \\
&\quad -\frac{\left(\left(4x_1^4+2x_1^2+1\right)x_2^2+3x_1^3x_2+x_1^2\right)\left(x_2x_1+1\right)}{2(x_2+x_1)^4} \\
&\quad +\frac{\left(2x_1^4+2x_1^3-x_1^2+1\right)\mathcal{D}_0(x_2)}{2(1+x_1)^2}-\frac{1-2x_2+2x_2^2}{2(1-x_1)}\Bigg], \qquad (5.67)
\end{aligned}
$$

$$
\mathcal{E}^0_{q\bar{q},q'} = (Q^2)^{-\epsilon}\frac{x_1\,x_2\,(1+x_1\,x_2)^2\,(1-x_1^2)}{2(x_1+x_2)^4}+(x_1\leftrightarrow x_2)\,, \qquad (5.68)
$$

$$
\begin{aligned}
\mathcal{E}_{qq',q} &= (Q^2)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{gq}(x_1)\delta(1-x_2) \\
&\quad +\frac{\mathcal{D}_0(x_2)\left(2-2x_1+x_1^2\right)}{2x_1}-\frac{x_1^2-2x_1+2}{2x_1(1-x_2)} \\
&\quad -\frac{x_2(x_1x_2+1)\left((x_1x_2-1)x_1^2+2\right)}{x_1(x_1+x_2)^2\left(x_2^2-1\right)} \\
&\quad +\frac{\left(2x_1+\left(2-2x_1+x_1^2\right)\log\left(\frac{2(1-x_1)}{x_1+1}\right)-2\right)\delta(1-x_2)}{2x_1}\Bigg], \qquad (5.69)
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{F}^0_{gg,g} &= -\mathbf{I}^{(1)}_{gg}(Q^2)\delta(1-x_1)\delta(1-x_2)+(Q^2)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{gg}(x_1)\delta(1-x_2) \\
&+\ \frac{1}{4}\pi^2\delta(1-x_1)\delta(1-x_2)+\left(-x_2^2+x_2-2+\frac{1}{x_2}\right)\mathcal{D}_0(x_1) \\
&+\ \delta(1-x_2)\mathcal{D}_1(x_1)+\left(\frac{1+\left(\log\left(\frac{2}{x_2+1}\right)-1\right)}{1-x_2}\right)\delta(1-x_1) \\
&-\ \left(\frac{\left(x_2^3-x_2^2+2x_2-1\right)\left(\log\left(2\frac{1-x_2}{x_2+1}\right)\right)}{x_2}\right)\delta(1-x_1) \\
&+\ \frac{1}{2}\mathcal{D}_0(x_1)\mathcal{D}_0(x_2)-\frac{3}{2(1+x_1)(1+x_2)}+\frac{2\left(x_1^4-x_1^2+2\right)\left(1+x_1x_2\right)^2}{(x_1+x_2)^4}+ \\
&+\ \frac{x_1^2-x_1+2+\frac{2}{(x_2+1)x_1}-\frac{1}{x_1}}{1-x_2}-\frac{2\left(x_1^4+x_1^2+\left(x_1^2+3\right)x_1+2\right)\left(1+x_1x_2\right)^2}{(1-x_2^2)(x_1+x_2)^4} \\
&+\ \frac{3\left(x_1^3+x_1\right)\left(x_2^3+x_2\right)\left(1+x_1x_2\right)}{(x_1+x_2)^4}+\frac{(1+x_1x_2)}{x_1(x_1+1)x_2(x_2+1)} \\
&+\ \frac{2x_1\left(x_1^2+3\right)\left(1+x_1x_2\right)^2}{(x_2+1)(x_1+x_2)^4}+\frac{2\left(x_2^2x_1^4+\left(x_2^2+1\right)^2x_1^2+x_2^2\right)\left(1+x_1x_2\right)}{(x_1+x_2)^4}\Bigg] \\
&+\ (x_1\leftrightarrow x_2)\,, \qquad (5.70)
\end{aligned}
$$

$$\begin{aligned}
\mathcal{G}^0_{q\bar{q},g} &= (Q^2)^{-\epsilon}\frac{(1+x_1\,x_2)x_1^2(1-x_2)^2(1+x_2)^2}{(x_1+x_2)^4} + (x_1 \leftrightarrow x_2)\,, &(5.71)\\
\mathcal{G}^0_{gq,q} &= (Q^2)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{gq}(x_1)\delta(1-x_2)\\
&\quad -\frac{\left(2(1-x_1)-(2-2x_1+x_1^2)\log\left(2\frac{1-x_1}{x_1+1}\right)\right)\delta(1-x_2)}{2x_1}\\
&\quad +\frac{\mathcal{D}_0(x_2)\,(2-2x_1+x_1^2)}{2x_1}-\frac{2-2x_1+x_1^2}{2x_1(1-x_2)}\\
&\quad +\frac{2(1+x_1x_2)\,(x_1^2+2x_2x_1+(x_1^4-2x_1^2+2)\,x_2^2)}{2x_1(x_1+x_2)^3\,(1-x_2^2)}\Bigg]\,. &(5.72)
\end{aligned}$$

# 5.6 Singular limits

In this section we list the singular limits of the antenna function described above. The soft and collinear limits of final-final antennae are already listed in ref. [20]; for completeness, we repeat them here. We also write down trivial limits for the same sake of completeness.

The limits are written in terms of the eikonal factor

$$S_{abc} = \frac{2s_{ac}}{s_{ab}s_{bc}}\,, \tag{5.73}$$

the final-final splitting functions

$$\begin{aligned}
P_{qg\to Q}(z) &= \frac{1+(1-z)^2-\epsilon z^2}{z},\\
P_{q\bar{q}\to G}(z) &= \frac{z^2+(1-z)^2-\epsilon}{1-\epsilon},\\
P_{gg\to G}(z) &= \frac{z}{1-z}+\frac{1-z}{z}+z(1-z)\,, &(5.74)
\end{aligned}$$

the initial-final splitting functions

$$\begin{aligned}
P_{gq\leftarrow Q}(z) &= \frac{1+z^2-\epsilon(1-z)^2}{(1-\epsilon)(1-z)^2} = \frac{1}{z}\frac{1}{1-\epsilon}P_{qg\to Q}(1-z),\\
P_{qg\leftarrow Q}(z) &= \frac{1+(1-z)^2-\epsilon z^2}{z(1-z)} = \frac{1}{1-z}P_{qg\to Q}(z),\\
P_{q\bar{q}\leftarrow G}(z) &= \frac{z^2+(1-z)^2-\epsilon}{1-z} = \frac{1-\epsilon}{1-z}P_{q\bar{q}\to G}(z),\\
P_{gg\leftarrow G}(z) &= \frac{2(1-z+z^2)^2}{z(1-z)^2} = \frac{1}{1-z}P_{gg\to G}(z)\,, &(5.75)
\end{aligned}$$

where $P_{ij\leftarrow K}$ is the splitting of the initial-state $K$ into parton $i$ entering the hard process and parton $j$ radiated. The definition of the momentum fraction $z$

changes depending on whether the particles becoming collinear are in the initial or in the final-state. For two final-state particles $p_1$ and $p_2$ becoming collinear in the direction $p_{12}$, we have the limits

$$p_1 \to zp_{12}, \quad p_2 \to (1-z)p_{12}, \quad s_{13} \to zs_{123}, \quad s_{23} \to (1-z)s_{123} \, , \tag{5.76}$$

whereas for a final-state particle $p_j$ becoming collinear with an initial-state parton $p_i$ we have

$$p_j \to zp_i, \quad p_{ij} \to (1-z)p_i, \quad s_{ik} \to \frac{s_{ijk}}{1-z}, \quad s_{jk} \to \frac{zs_{ijk}}{1-z} \, . \tag{5.77}$$

This explains the difference between final-final and initial-final splitting functions. For collinear singularities between an initial $p_i$ and a final-state parton $p_k$, the limits are proportional to the propagator going onshell, namely $1/(1-z)s_{ik}$, whereas for two final-state partons $p_j$ and $p_k$ the limit is proportional to $s_{jk}$, therefore the factor $1-z$ in the initial-final splittings. The factors of $1-\epsilon$ or $1/(1-\epsilon)$ account for the different number of polarizations when the type of particle entering the hard process is changed.

### 5.6.1 Final-final antennae

The final-final antennae can have soft limits when one gluon becomes soft, or when any two partons become collinear.

The quark-antiquark antenna $A(1_q, 3_g, 2_{\bar{q}})$ have a non vanishing soft limit when the gluon becomes soft. Non-vanishing collinear limits are obtained when the gluon becomes collinear to one of the hard radiators.

$$A_{qg\bar{q}}(1,3,2) \overset{3_g \to 0}{\longrightarrow} S_{132} \tag{5.78}$$

$$A_{qg\bar{q}}(1,3,2) \overset{3_g \| 1_q}{\longrightarrow} \frac{1}{s_{13}} P_{qg\to Q}(z) \tag{5.79}$$

$$A_{qg\bar{q}}(1,3,2) \overset{3_g \| 2_q}{\longrightarrow} \frac{1}{s_{23}} P_{qg\to Q}(z) \tag{5.80}$$

$$A_{qg\bar{q}}(1,3,2) \overset{1_q \| 2_q}{\longrightarrow} 0 \tag{5.81}$$

$$\tag{5.82}$$

The quark-gluon antenna $D_{qgg}(1,2,3)$ has a non-vanishing soft limit when one of the gluons becomes soft. Non-vanishing collinear limits are obtained in all collinear configurations.

$$D_{qgg}(1,2,3) \stackrel{2_g\to 0}{\longrightarrow} S_{123} \tag{5.83}$$
$$D_{qgg}(1,2,3) \stackrel{3_g\to 0}{\longrightarrow} S_{132} \tag{5.84}$$

$$D_{qgg}(1,2,3) \stackrel{2_g\|1_q}{\longrightarrow} \frac{1}{s_{12}}P_{qg\to Q}(z) \tag{5.85}$$
$$D_{qgg}(1,2,3) \stackrel{3_g\|1_q}{\longrightarrow} \frac{1}{s_{13}}P_{qg\to Q}(z) \tag{5.86}$$
$$D_{qgg}(1,2,3) \stackrel{2_g\|3_g}{\longrightarrow} \frac{1}{s_{23}}P_{gg\to G}(z) \tag{5.87}$$
$$\tag{5.88}$$

The quark-gluon antenna $E_{qq'\bar{q}'}(1,3,4)$ has no soft limits (since there are no final-state gluons). Non-vanishing collinear limits appear when the two quarks/antiquarks of the same type become collinear.

$$E_{qq'\bar{q}'}(1,2,3) \stackrel{2_{q'}\|3_{\bar{q}'}}{\longrightarrow} \frac{1}{s_{23}}P_{q\bar{q}\to G}(z) \tag{5.89}$$
$$E_{qq'\bar{q}'}(1,2,3) \stackrel{1_q\|2_{q'}}{\longrightarrow} 0 \tag{5.90}$$
$$E_{qq'\bar{q}'}(1,2,3) \stackrel{1_q\|3_{\bar{q}'}}{\longrightarrow} 0 \tag{5.91}$$
$$\tag{5.92}$$

The gluon-gluon antenna $F_{ggg}(1,2,3)$ has soft limits for each gluon becoming soft. Non vanishing collinear limits appear when two gluons become collinear.

$$F_{ggg}(1,2,3) \stackrel{2_g\to 0}{\longrightarrow} S_{123} \tag{5.93}$$
$$F_{ggg}(1,2,3) \stackrel{3_g\to 0}{\longrightarrow} S_{132} \tag{5.94}$$
$$F_{ggg}(1,2,3) \stackrel{1_g\to 0}{\longrightarrow} S_{213} \tag{5.95}$$

$$F_{ggg}(1,2,3) \stackrel{2_g\|1_g}{\longrightarrow} \frac{1}{s_{12}}P_{gg\to G}(z) \tag{5.96}$$
$$F_{ggg}(1,2,3) \stackrel{3_g\|1_g}{\longrightarrow} \frac{1}{s_{13}}P_{gg\to G}(z) \tag{5.97}$$
$$F_{ggg}(1,2,3) \stackrel{2_g\|3_g}{\longrightarrow} \frac{1}{s_{23}}P_{gg\to G}(z) \tag{5.98}$$

The gluon-gluon antenna $G_{gq\bar{q}}(1,3,4)$ has only one non-vanishing collinear limit, when the quark-antiquark pair becomes collinear.

$$G_{gq\bar{q}}(1,2,3) \xrightarrow{2_q\|3_{\bar{q}}} \frac{1}{s_{23}} P_{q\bar{q}\to G}(z) \tag{5.99}$$

$$G_{gq\bar{q}}(1,2,3) \xrightarrow{1_g\|2_q} 0 \tag{5.100}$$

$$G_{gq\bar{q}}(1,2,3) \xrightarrow{1_g\|3_{\bar{q}}} 0 \tag{5.101}$$

$$\tag{5.102}$$

### 5.6.2 Initial-final antennae

The initial-final antennae $\mathcal{X}_{i,jk}$ can have non-vanishing soft and collinear singular limits when one of the two final-state momenta $j$ or $k$ becomes soft, when one of them becomes collinear to the initial-state parton $i$ or when both final-state partons become collinear.

The initial-final quark-antiquark antenna $A_{q,gq}(1;3,2)$ has a non vanishing soft limit when the gluon becomes soft and non vanishing collinear limits when the gluon becomes collinear to either the initial- or final-state quark. It vanishes in the case where the initial and final quark become collinear.

$$A_{q,gq}(1_q;3_g,2_q) \xrightarrow{3_g\to 0} S_{132} \tag{5.103}$$

$$A_{q,gq}(1;3,2) \xrightarrow{3_g\|1_q} \frac{1}{s_{13}} P_{qg\leftarrow Q}(z) \tag{5.104}$$

$$A_{q,gq}(1;3,2) \xrightarrow{3_g\|2_q} \frac{1}{s_{23}} P_{qg\to Q}(z) \tag{5.105}$$

$$A_{q,gq}(1;3,2) \xrightarrow{1_q\|2_q} 0 \tag{5.106}$$

The initial-final quark-antiquark antenna $A_{g,q\bar{q}}(3;1,2)$ has no vanishing soft limit since the gluon is in the initial-state; it has non-vanishing collinear limits when one of the final-state partons becomes collinear with the initial-state gluon but no collinear limit in the case where the quark and the antiquark become collinear.

$$A_{g,q\bar{q}}(3;1,2) \xrightarrow{1_q\|3_g} \frac{1}{s_{13}} P_{q\bar{q}\leftarrow G}(z) \tag{5.107}$$

$$A_{g,q\bar{q}}(3;1,2) \xrightarrow{2_{\bar{q}}\|3_g} \frac{1}{s_{23}} P_{q\bar{q}\leftarrow G}(z) \tag{5.108}$$

$$A_{g,q\bar{q}}(3;1,2) \xrightarrow{2_{\bar{q}}\|1_q} 0 \tag{5.109}$$

The quark-induced initial-final quark-gluon antenna $D_{q,gg}(1;2,3)$ has a non-vanishing soft limit when one of the final-state gluon becomes soft and non-vanishing collinear limits in all the kinematically unsuppressed configurations,

$$D_{q,gg}(1;2,3) \xrightarrow{3_g\to 0} S_{123} \tag{5.110}$$
$$D_{q,gg}(1;2,3) \xrightarrow{2_g\to 0} S_{132} \tag{5.111}$$

$$D_{q,gg}(1;2,3) \xrightarrow{2_g\|1_q} \frac{1}{s_{12}}P_{qg\leftarrow Q}(z) \tag{5.112}$$
$$D_{q,gg}(1;2,3) \xrightarrow{3_g\|1_q} \frac{1}{s_{13}}P_{qg\leftarrow Q}(z) \tag{5.113}$$
$$D_{q,gg}(1;2,3) \xrightarrow{2_g\|3_g} \frac{1}{s_{23}}P_{gg\to G}(z) \tag{5.114}$$
$$\tag{5.115}$$

The gluon-induced initial-final quark-gluon antenna is split into two contributions $D_{g,qg}(2;1,3)$ and $D_{g,gq}(2;3,1)$ so that the first contains only the collinear limit of the quark becoming collinear to the initial-state gluon and the latter containing both the soft limit of the final-state gluon and its collinear limit with the initial-state gluon,

$$D_{g,qg}(2;1,3) \xrightarrow{3_g\to 0} 0 \tag{5.116}$$

$$D_{g,qg}(2;1,3) \xrightarrow{1_q\|2_g} \frac{1}{s_{12}}P_{q\bar{q}\leftarrow G}(z) \tag{5.117}$$
$$D_{g,qg}(2;1,3) \xrightarrow{1_q\|3_g} 0 \tag{5.118}$$
$$D_{g,qg}(2;1,3) \xrightarrow{2_g\|3_g} 0 \tag{5.119}$$

$$D_{g,gq}(2;3,1) \xrightarrow{3_g\to 0} S_{132} \tag{5.120}$$

$$D_{g,gq}(2;3,1) \xrightarrow{1_q\|3_g} \frac{1}{s_{13}}P_{qg\to Q}(z) \tag{5.121}$$
$$D_{g,gq}(2;3,1) \xrightarrow{2_g\|3_g} \frac{1}{s_{23}}P_{gg\leftarrow G}(z) \tag{5.122}$$
$$D_{g,gq}(2;3,1) \xrightarrow{1_q\|2_g} 0 \tag{5.123}$$

The initial-final quark-gluon antennae with two different quark types $E_{q,q'\bar{q}'}(1;2,3)$ and $E_{q',qq'}(3;1,2)$ have no soft limit (as they have no gluons) and only collinear limits when the two quarks of the same type become collinear,

$$E_{q,q'\bar{q}'}(1;2,3) \xrightarrow{2_{q'}\|3_{\bar{q}'}} \frac{1}{s_{23}} P_{q\bar{q}\to G}(z) \tag{5.124}$$
$$E_{q,q'\bar{q}'}(1;2,3) \xrightarrow{1_q\|2_{q'}} 0 \tag{5.125}$$
$$E_{q,q'\bar{q}'}(1;2,3) \xrightarrow{1_q\|3_{\bar{q}'}} 0 \tag{5.126}$$

$$E_{q',qq'}(3;1,2) \xrightarrow{2_{q'}\|3_{\bar{q}'}} \frac{1}{s_{23}} P_{gq\leftarrow Q}(z) \tag{5.127}$$
$$E_{q',qq'}(3;1,2) \xrightarrow{1_q\|2_{q'}} 0 \tag{5.128}$$
$$E_{q',qq'}(3;1,2) \xrightarrow{1_q\|3_{\bar{q}'}} 0 \tag{5.129}$$

The initial-final gluon-gluon antennae $F_{g,gg}(1;2,3)$ has soft limits when one of the final-state gluons becomes soft, and non-vanishing collinear limit when any two gluons become collinear,

$$F_{g,gg}(1;2,3) \xrightarrow{2_g\to 0} S_{123} \tag{5.130}$$
$$F_{g,gg}(1;2,3) \xrightarrow{3_g\to 0} S_{132} \tag{5.131}$$

$$F_{g,gg}(1;2,3) \xrightarrow{2_g\|1_g} \frac{1}{s_{12}} P_{gg\leftarrow G}(z) \tag{5.132}$$
$$F_{g,gg}(1;2,3) \xrightarrow{3_g\|1_g} \frac{1}{s_{13}} P_{gg\leftarrow G}(z) \tag{5.133}$$
$$F_{g,gg}(1;2,3) \xrightarrow{2_g\|3_g} \frac{1}{s_{23}} P_{gg\to G}(z) \tag{5.134}$$

The initial-final gluon-gluon antennae $G_{q,gq}(3_q;1_g,2_q)$ and $G_{g,q\bar{q}}(1_g;2_q,3_{\bar{q}})$ have no soft limits and only one non-vanishing collinear limit when the quark and antiquark become colinear.

$$G_{q,gq}(3;1,2) \xrightarrow{2_q\|3_q} \frac{1}{s_{23}} P_{gq\leftarrow Q}(1) \tag{5.135}$$
$$G_{q,gq}(3;1,2) \xrightarrow{1_g\|2_q} 0 \tag{5.136}$$
$$G_{q,gq}(3;1,2) \xrightarrow{1_g\|3_q} 0 \tag{5.137}$$

$$G_{g,q\bar{q}}(1;2,3) \xrightarrow{2_q\|3_{\bar{q}}} \frac{1}{s_{23}} P_{q\bar{q}\to G}(z) \tag{5.138}$$
$$G_{g,q\bar{q}}(1;2,3) \xrightarrow{1_g\|2_q} 0 \tag{5.139}$$
$$G_{g,q\bar{q}}(1;2,3) \xrightarrow{1_g\|3_{\bar{q}}} 0 \tag{5.140}$$

### 5.6.3 Initial-initial antennae

The initial-initial antennae $\mathcal{X}_{ij,k}$ only have singular limits when particle $k$ becomes collinear to $i$ or $j$, or when it becomes soft. The other possibilities are kinematically suppressed.

The initial-initial quark-antiquark antenna $A_{qg,q}(1,3;2)$ has no soft limit and one collinear limit,

$$A_{qg,q}(1,3;2) \quad \stackrel{2_q\|3_g}{\longrightarrow} \quad \frac{1}{s_{23}} P_{q\bar{q}\leftarrow G}(z) \tag{5.141}$$

$$A_{qg,q}(1,3;2) \quad \stackrel{2_q\|1_q}{\longrightarrow} \quad 0 \tag{5.142}$$

The initial-initial quark-antiquark antenna $A_{q\bar{q},g}(1,2;3)$ has one soft limit and two collinear limits when the final-state gluon becomes collinear with one of the initial-state partons,

$$A_{q\bar{q},g}(1,2;3) \quad \stackrel{3_g\to 0}{\longrightarrow} \quad S_{132} \tag{5.143}$$

$$A_{q\bar{q},g}(1,2;3) \quad \stackrel{3_g\|1_q}{\longrightarrow} \quad \frac{1}{s_{13}} P_{qg\leftarrow Q}(z) \tag{5.144}$$

$$A_{q\bar{q},g}(1,2;3) \quad \stackrel{3_g\|2_{\bar{q}}}{\longrightarrow} \quad \frac{1}{s_{23}} P_{qg\leftarrow Q}(z) \tag{5.145}$$

The initial-initial quark-gluon antenna $D_{gg,q}(2,3;1)$ has only collinear limits,

$$D_{gg,q}(2,3;1) \quad \stackrel{1_q\|2_g}{\longrightarrow} \quad \frac{1}{s_{12}} P_{q\bar{q}\leftarrow G}(z) \tag{5.146}$$

$$D_{gg,q}(2,3;1) \quad \stackrel{1_q\|3_g}{\longrightarrow} \quad \frac{1}{s_{13}} P_{q\bar{q}\leftarrow G}(z) \tag{5.147}$$

whereas $D_{qg,g}(1,2;3)$ has both soft and collinear non-vanishing limits,

$$D_{qg,g}(1,2;3) \quad \stackrel{3_g\to 0}{\longrightarrow} \quad S_{132} \tag{5.148}$$

$$D_{qg,g}(1,2;3) \quad \stackrel{3_g\|2_g}{\longrightarrow} \quad \frac{1}{s_{23}} P_{gg\leftarrow G}(z) \tag{5.149}$$

$$D_{qg,g}(1,2;3) \quad \stackrel{3_g\|1_q}{\longrightarrow} \quad \frac{1}{s_{13}} P_{qg\leftarrow Q}(z). \tag{5.150}$$

The initial-initial quark-gluon antenna $E_{q\bar{q},q'}(2,3;1)$ has no singular limits,

$$E_{q\bar{q},q'}(2,3;1) \quad \stackrel{1_{\bar{q}}\to 0}{\longrightarrow} \quad 0 \tag{5.151}$$

$$E_{q\bar{q},q'}(2,3;1) \quad \stackrel{1_q\|2_{q'}}{\longrightarrow} \quad 0 \tag{5.152}$$

$$E_{q\bar{q},q'}(2,3;1) \quad \stackrel{1_q\|3_{\bar{q}'}}{\longrightarrow} \quad 0 \tag{5.153}$$

whereas $E_{qq',q}(1,2;3)$ has a non vanishing collinear limit when the final-state quark is collinear to the initial quark of the same type,

$$E_{qq',q}(1,2;3) \xrightarrow{2_{q'}\|3_{\bar{q}'}} \frac{1}{s_{23}}P_{gq\leftarrow Q}(z) \tag{5.154}$$

$$E_{qq',q}(1,2;3) \xrightarrow{1_q\|3_{\bar{q}'}} 0 \tag{5.155}$$

The initial-initial gluon-gluon antenna $F_{ggg}(1,2;3)$ has both soft and collinear limits,

$$F_{ggg}(1,2;3) \xrightarrow{3_g\to 0} S_{123} \tag{5.156}$$

$$F_{ggg}(1,2;3) \xrightarrow{3_g\|1_g} \frac{1}{s_{13}}P_{gg\leftarrow G}(z) \tag{5.157}$$

$$F_{ggg}(1,2;3) \xrightarrow{3_g\|2_g} \frac{1}{s_{23}}P_{gg\leftarrow G}(z) \tag{5.158}$$

The initial-initial gluon-gluon antennae $G_{gq,q}(1,2;3)$ and $G_{q\bar{q},g}(2,3;1)$ have collinear limits but no soft limits,

$$G_{gq,q}(1,2;3) \xrightarrow{2_q\|3_q} \frac{1}{s_{23}}P_{gq\to Q}(z) \tag{5.159}$$

$$G_{gq,q}(1,2;3) \xrightarrow{1_g\|3_q} 0 \tag{5.160}$$

$$G_{q\bar{q},g}(2,3;1) \xrightarrow{1_g\to 0} 0 \tag{5.161}$$

$$G_{q\bar{q},g}(2,3;1) \xrightarrow{1_g\|2_q} 0 \tag{5.162}$$

$$G_{q\bar{q},g}(2,3;1) \xrightarrow{1_g\|3_{\bar{q}}} 0 \tag{5.163}$$

## 5.7 Application of method at NLO

To illustrate the application of the antenna subtraction method at NLO, we derive the antenna subtraction terms for two example reactions: deep inelastic (2+1)-jet production and hadronic vector-boson-plus-jet production. Several NLO calculations are already available in the literature both for DIS jet production [5, 40, 41] and for vector boson production [4].

### 5.7.1 (2+1)-jet production in deep inelastic scattering

The production of (2+1) jets in deep inelastic lepton-proton scattering can be described on the parton level by the scattering of a space-like virtual gauge boson and a parton, yielding a final-state with two hard partons (with the extra jet coming from the proton remnant, not participating in the hard interaction). We limit ourselves to consider the scattering of transversely polarized virtual photons. The cross section can be written as

$$d\sigma = \int \frac{d\xi}{\xi} \sum_q f_q(\xi)\, \mathrm{d}\hat{\sigma}_q + f_g(\xi)\, \mathrm{d}\hat{\sigma}_g\,. \tag{5.164}$$

The partonic cross sections up to NLO are, in turn, given by,

$$\begin{aligned}
\mathrm{d}\hat{\sigma}_q \;=\;& \mathrm{d}\Phi_2(k_g, k_q; p_q, q)\, \left|M^0_{q,gq}\right|^2\, J_2^{(2)}(k_g, k_q) \\
&+\mathrm{d}\Phi_2(k_g, k_q; p_q, q)\, 2\Re(M^{1\dagger}_{q,gq} M^0_{q,gq})\, J_2^{(2)}(k_g, k_q) \\
&+\mathrm{d}\Phi_3(k_{g_1}, k_{g_2}, k_q; p_q, q)\, \left|M^0_{q,ggq}\right|^2\, J_2^{(3)}(k_{g_1}, k_{g_2}, k_q) \\
&+\mathrm{d}\Phi_3(k_{q_1}, k_{q_2}, k_{\bar{q}}; p_q, q)\, \left|M^0_{q,qq\bar{q}}\right|^2\, J_2^{(3)}(k_q, k_q, k_{\bar{q}}) \\
&+\sum_{q'\neq q} \mathrm{d}\Phi_3(k_q, k_{q'}, k_{\bar{q}'}; p_q, q)\, \left|M^0_{q,qq'\bar{q}'}\right|^2\, J_2^{(3)}(k_q, k_{q'}, k_{\bar{q}'})\,, \qquad (5.165) \\
\mathrm{d}\hat{\sigma}_g \;=\;& \mathrm{d}\Phi_2(k_q, k_{\bar{q}}; p_g, q)\, \left|M^0_{g,q\bar{q}}\right|^2\, J_2^{(2)}(k_q, k_{\bar{q}}) \\
&+\mathrm{d}\Phi_2(k_q, k_{\bar{q}}; p_q, q)\, 2\Re(M^{1\dagger}_{g,q\bar{q}} M^0_{g,q\bar{q}})\, J_2^{(2)}(k_q, k_{\bar{q}}) \\
&+\mathrm{d}\Phi_3(k_g, k_q, k_{\bar{q}}; p_q, q)\, \left|M^0_{g,gq\bar{q}}\right|^2\, J_2^{(3)}(k_g, k_q, k_{\bar{q}})\,. \qquad (5.166)
\end{aligned}$$

For the sake of brevity, the momentum arguments on the matrix elements are omitted. The first index on the matrix elements indicates the incoming parton, the remaining ones the outgoing partons. Subtractions for infrared real radiation singularities must be performed only on the three-parton final-states. The matrix elements for the real contributions can be expressed in terms of colour-ordered three-parton and four-parton antenna functions. They read as follows:

$$\begin{aligned}
\left|M^0_{q,gq}\right|^2 \;=\;& e_q^2\, N_{2,q}\, A_3^0(1_q, 3_g, \hat{2}_{\bar{q}}) \qquad (5.167) \\
\left|M^0_{q,ggq}\right|^2 \;=\;& e_q^2\, \frac{1}{2}\, N_{3,q} \Bigg[ N\, A_4^0(1_q, 3_g, 4_g, \hat{2}_{\bar{q}}) + N\; A_4^0(1_q, 4_g, 3_g, \hat{2}_{\bar{q}}) \\
&\qquad - \frac{1}{N}\, \tilde{A}_4^0(1_q, 3_g, 4_g, \hat{2}_{\bar{q}}) \Bigg]\,, \qquad (5.168) \\
\left|M^0_{q,qq\bar{q}}\right|^2 + \left|M^0_{q,qq'\bar{q}'}\right|^2 \;=\;& e_q^2\, N_{3,q} \Bigg[ N_F\, B_4^0(1_q, 3_{q'}, 4_{\bar{q}'}, \hat{2}_{\bar{q}}) \\
&- \frac{1}{N} \big( C_4^0(1_q, 3_q, 4_{\bar{q}}, \hat{2}_{\bar{q}}) + C_4^0(1_q, 3_q, \hat{2}_{\bar{q}}, 4_{\bar{q}}) \\
&\qquad + C_4^0(4_{\bar{q}}, \hat{2}_{\bar{q}}, 1_q, 3_q) + C_4^0(\hat{2}_{\bar{q}}, 4_{\bar{q}}, 1_q, 3_q) \big) \Bigg] \\
&+ \sum_{q'} e_{q'}^2\, N_{3,q}\, B_4^0(3_{q'}, 1_q, \hat{2}_{\bar{q}}, 4_{\bar{q}'})\,, \qquad (5.169)
\end{aligned}$$

$$\begin{aligned}
\left|M^0_{g,q\bar{q}}\right|^2 &= \sum_q e_q^2\, N_{2,g}\; A_4^0(1_q,\hat{3}_g,2_{\bar{q}})\,, && (5.170)\\
\left|M^0_{g,gq\bar{q}}\right|^2 &= \sum_q e_q^2\, N_{3,g}\left[N\, A_4^0(1_q,\hat{3}_g,4_g,2_{\bar{q}}) + N\, A_4^0(1_q,4_g,\hat{3}_g,2_{\bar{q}})\right.\\
&\qquad\left. -\frac{1}{N}\,\tilde{A}_4^0(1_q,\hat{3}_g,4_g,2_{\bar{q}})\right]\,, && (5.171)
\end{aligned}$$

where

$$N_{n,q} = 4\,\pi\alpha\,(g^2)^{n-2}\frac{N^2-1}{N}\,2\,(1-\epsilon)\,Q^2\,, \qquad (5.172)$$

and

$$N_{n,g} = 4\,\pi\alpha\,(g^2)^{n-2}\,2\,Q^2\,. \qquad (5.173)$$

All the antenna functions used here can be obtained from explicit expressions for the final-final antennae $X_3^0$ and $X_4^0$ in ref. [20] by crossing in each case the particle denoted by $\hat{n}_i$.

The subtraction terms for both quark and gluon initiated processes are a combination of final-final and initial-final subtractions. We split the quark-induced contributions into three terms: quark-plus-two-gluon final-states at leading and subleading colour, $\mathrm{d}\hat{\sigma}^S_{q,A}$ and $\mathrm{d}\hat{\sigma}^S_{q,\tilde{A}}$ and quark-quark-antiquark final-state $\mathrm{d}\hat{\sigma}^S_{q,B}$. Identical-only quark contributions to the matrix elements, involving the antenna $C_4^0$, have no single collinear limits so they do not need to be subtracted. Gluon-induced contributions can also be split into leading and subleading colour, $\mathrm{d}\hat{\sigma}^S_{g,A}$ and $\mathrm{d}\hat{\sigma}^S_{g,\tilde{A}}$. The explicit expressions for subtraction terms are given by

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q,A} = &\quad e_q^2\, N_{3,q}\mathrm{d}\Phi_3(k_{g_1},k_{g_2},k_q;p_q,q)\frac{N}{2}\\
&\times\Big(D^0_{q,g_1g_2}\,A^0_{Q,Gq}\,J_2^{(2)}(K_G,k_q) + D^0_{g_1g_2q}A^0_{q,GQ}\,J_2^{(2)}(K_G,K_Q)\Big)\,, && (5.174)\\
\mathrm{d}\hat{\sigma}^S_{q,\tilde{A}} = & -e_q^2\, N_{3,q}\mathrm{d}\Phi_3(k_{g_1},k_{g_2},k_q;p_q,q)\frac{1}{2N}\\
&\times\Big(A^0_{q,g_1q}\,A^0_{Q,g_2Q}\,J_2^{(2)}(k_{g_2},K_Q) + A^0_{q,g_2q}\,A^0_{Q,g_1,Q}\,J_2^{(2)}(k_{g_1},K_Q)\Big) && (5.175)\\
\mathrm{d}\hat{\sigma}^S_{q,B} = &\quad N_{3,q}\mathrm{d}\Phi_3(k_q,k_{q'},k_{\bar{q}'};p_q,q)\left[\sum_{q'} e_{q'}^2\,E^0_{q,qq'}\,A^0_{G,Q'\bar{q}'}\,J_2^{(2)}(K_{Q'},k_{\bar{q}'})\right.\\
&\left.+\frac{N_F}{2}\,e_q^2\,\Big(E^0_{q,q'\bar{q}'}\,A^0_{Q,Gq}\,J_2^{(2)}(K_G,k_q) + E^0_{qq'\bar{q}'}\,A^0_{q,GQ}\,J_2^{(2)}(K_G,k_q)\Big)\right]\,,\\
& && (5.176)
\end{aligned}$$

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{g,A} = \quad & \sum_q e_q^2\, N_{3,g} \mathrm{d}\Phi_3(k_g,k_q,k_{\bar{q}};p_g,q)\, N \\
& \times \Big( D^0_{g,\bar{q}g}\, A^0_{Q,Gq}\, J_2^{(2)}(K_G,k_q) + D^0_{g,g\bar{q}} A^0_{G,q,\bar{Q}}\, J_2^{(2)}(k_q,K_{\bar{Q}}) \\
& \quad + D^0_{g,qg}\, A^0_{\bar{Q},G\bar{q}}\, J_2^{(2)}(K_G,k_{\bar{q}}) + D^0_{g,gq} A^0_{G,Q\bar{q}}\, J_2^{(2)}(K_Q,k_{\bar{q}}) \Big) \quad (5.177) \\
\mathrm{d}\hat{\sigma}^S_{g,\tilde{A}} = \quad & -\sum_q e_q^2\, N_{3,g} \mathrm{d}\Phi_3(k_g,k_q,k_{\bar{q}};p_g,q) \frac{1}{N} \\
& \times \Big( \frac{1}{2} A^0_{g,q\bar{q}}\, A^0_{Q,gQ}\, J_2^{(2)}(k_g,K_Q) + \frac{1}{2} A^0_{g,q\bar{q}}\, A^0_{\bar{Q},g\bar{Q}}\, J_2^{(2)}(k_g,K_{\bar{Q}}) \\
& + A^0_{qg\bar{q}} A^0_{g,Q\bar{Q}}\, J_2^{(2)}(K_Q,K_{\bar{Q}}) \Big) . \quad (5.178)
\end{aligned}
$$

In the above, $X_{I,Jk}$ and $X_{k,IJ}$ denote three-parton antenna functions with momenta $I, J$ obtained from a phase space mapping. The combination of these subtraction terms with the real matrix elements containing three partons in the final-state is finite in all soft and collinear limits and can be integrated numerically over the three-particle phase space.

On the other hand, the analytical integration of the subtraction terms over the factorized phase space can be carried out using the results of Section 5.4.3. For the poles of the integrated terms, we obtain:

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q,A} + \mathrm{d}\hat{\sigma}^S_{q,\tilde{A}} + \mathrm{d}\hat{\sigma}^S_{q,B} \; = \; & -2\,\frac{\alpha_s}{2\pi} \Big[ N \, \left( \mathbf{I}^{(1)}_{qg}(t) + \mathbf{I}^{(1)}_{qg}(s) \right) - \frac{1}{N}\, \mathbf{I}^{(1)}_{q\bar{q}}(u) \\
& \qquad + N_F \, \left( \mathbf{I}^{(1)}_{qg,F}(t) + \mathbf{I}^{(1)}_{qg,F}(s) \right) \Big] \, \mathrm{d}\hat{\sigma}^B_q(p,q) \\
& - \frac{\alpha_s}{2\pi} \int \frac{dx}{x} \frac{1}{\epsilon}\, C_F\, p^{(0)}_{qq}(x)\, \mathrm{d}\hat{\sigma}^B_q(xp,q) \\
& - \frac{\alpha_s}{2\pi} \int \frac{dx}{x} \frac{1}{\epsilon}\, C_F\, p^{(0)}_{gq}(x)\, \mathrm{d}\hat{\sigma}^B_g(xp,q) + \mathcal{O}(\epsilon^0) , \qquad (5.179) \\
\mathrm{d}\hat{\sigma}^S_{g,A} + \mathrm{d}\hat{\sigma}^S_{g,\tilde{A}} \; = \; & -2\,\frac{\alpha_s}{2\pi} \Big[ N \, \left( \mathbf{I}^{(1)}_{qg}(t) + \mathbf{I}^{(1)}_{qg}(u) \right) - \frac{1}{N}\, \mathbf{I}^{(1)}_{q\bar{q}}(s) \\
& \qquad + N_F \, \left( \mathbf{I}^{(1)}_{qg,F}(t) + \mathbf{I}^{(1)}_{qg,F}(u) \right) \Big] \, \mathrm{d}\hat{\sigma}^B_g(p,q) \\
& - \frac{\alpha_s}{2\pi} \int \frac{dx}{x} \frac{1}{\epsilon} \left( N\, p^{(0)}_{gg}(x) + N_F\, p^{(0)}_{gg,F}(x) \right) \, \mathrm{d}\hat{\sigma}^B_g(xp,q) \\
& - \frac{\alpha_s}{2\pi} \int \frac{dx}{x} \frac{1}{\epsilon}\, T_F\, p^{(0)}_{qg}(x) \, \left( \mathrm{d}\hat{\sigma}^B_q(xp,q) + \mathrm{d}\hat{\sigma}^B_{\bar{q}}(xp,q) \right) + \mathcal{O}(\epsilon^0) , \\
& \qquad (5.180)
\end{aligned}
$$

where $C_F = (N^2-1)/(2N)$, $T_F = \frac{1}{2}$ and the Born cross sections are given by

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^B_q(p,q) &= \mathrm{d}\Phi_2(k_g,k_q;p,q)\, \left| M^0_{q,gq} \right|^2 \, J_2^{(2)}(k_g,k_q), \qquad (5.181) \\
\mathrm{d}\hat{\sigma}^B_g(p,q) &= \mathrm{d}\Phi_2(k_q,k_{\bar{q}};p,q)\, \left| M^0_{g,q\bar{q}} \right|^2 \, J_2^{(2)}(k_q,k_{\bar{q}}). \qquad (5.182)
\end{aligned}
$$

The poles contained in the operators $\mathbf{I}_{ij}^{(1)}$ match exactly the ones appearing, with opposite sign, in the interference of the renormalized one loop amplitudes with the Born ones. The remaining poles correspond to the mass-factorization contributions. Thus, combining the integrated subtraction terms with the virtual contributions and the mass-factorization counterterms, we obtain a finite contribution, free of any poles in $\epsilon$, that can be integrated over the two-parton phase space.

### 5.7.2 Vector-boson-plus-jet production in hadronic colliders

The second example we will consider is the production of a vector boson $V$ ($V = \gamma$, $Z$, $W^{\pm}$) plus a hadronic jet in a hadronic collision. This process is mediated by the scattering of two partons into the vector boson and one hard parton. The cross section is given by

$$
\begin{aligned}
d\sigma \;=\; \int \frac{d\xi_1}{\xi_1}\frac{d\xi_2}{\xi_2} \Big\{ & \sum_{i,j} \left[f_{q_i}(\xi_1) f_{\bar{q}_j}(\xi_2) + f_{\bar{q}_i}(\xi_1) f_{q_j}(\xi_2)\right] \mathrm{d}\hat{\sigma}_{q_i\bar{q}_j} \\
& + \sum_{i,j} \left[f_{q_i}(\xi_1) f_{q_j}(\xi_2) + f_{\bar{q}_i}(\xi_1) f_{\bar{q}_j}(\xi_2)\right] \mathrm{d}\hat{\sigma}_{q_i q_j} \\
& + \sum_{i} \left[\left(f_{q_i}(\xi_1) + f_{\bar{q}_i}(\xi_1)\right) f_g(\xi_2) + f_g(\xi_1)\left(f_{q_i}(\xi_2) + f_{\bar{q}_i}(\xi_2)\right)\right] \mathrm{d}\hat{\sigma}_{q_i g} \\
& + f_g(\xi_1) f_g(\xi_2)\, \mathrm{d}\hat{\sigma}_{gg} \Big\}\, .
\end{aligned} \tag{5.183}
$$

Again we express the partonic cross sections in terms of color ordered antennae. We first write:

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}_{q_i\bar{q}_j} \;=\; & \mathrm{d}\Phi_2(k_g, q; p_q, p_{\bar{q}}) \left|M^0_{q_i\bar{q}_j,g}\right|^2 J_1^{(1)}(k_g) \\
& + \mathrm{d}\Phi_2(k_g, q; p_q, p_{\bar{q}})\, 2\Re(M^{1\dagger}_{q_i\bar{q}_j,g} M^0_{q_j\bar{q}_j,g})\, J_1^{(1)}(k_g) \\
& + \mathrm{d}\Phi_3(k_{g_1}, k_{g_2}, q; p_q, p_{\bar{q}}) \left|M^0_{q_i\bar{q}_j,gg}\right|^2 J_1^{(2)}(k_{g_1}, k_{g_2}) \\
& + \sum_{k,l} \mathrm{d}\Phi_2(k_q, k_{\bar{q}}, q; p_q, p_{\bar{q}}) \left|M^0_{q_i\bar{q}_j,q_k\bar{q}_l}\right|^2 J_1^{(2)}(k_{q_3}, k_{\bar{q}_4})\, ,
\end{aligned} \tag{5.184}
$$

$$
\mathrm{d}\hat{\sigma}_{q_i q_j} \;=\; \sum_{k,l} \mathrm{d}\Phi_3(k_{q_k}, k_{q_l}, q; p_{q_i}, p_{q_j}) \left|M^0_{q_i q_j,q_k q_l}\right|^2 J_1^{(2)}(k_{q_3}, k_{q_4})\, , \tag{5.185}
$$

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}_{q_i g} &= \sum_j \mathrm{d}\Phi_2(k_q, q; p_q, p_g) \left|M^0_{q_i g, q_j}\right|^2 J_1^{(1)}(k_q) \\
&+ \sum_j \mathrm{d}\Phi_2(k_q, q; p_q, p_g)\, 2\Re(M^{1\dagger}_{q_i g, q_j} M^0_{q_i g, q_j})\, J_1^{(2)}(k_q) \\
&+ \sum_j \mathrm{d}\Phi_3(k_q, k_g, q; p_q, p_g) \left|M^0_{q_i g, q_j g}\right|^2 J_1^{(2)}(k_q, k_g) \\
\mathrm{d}\hat{\sigma}_{gg} &= \sum_{i,j} \mathrm{d}\Phi_3(k_q, k_{\bar{q}}, q; p_{g_1}, p_{g_2}) \left|M^0_{gg, q_i\bar{q}_j}\right|^2 J_1^{(2)}(k_q, k_{\bar{q}})\,, \qquad (5.186)
\end{aligned}
$$

where we have omitted again the momentum arguments of the matrix elements. The matrix element for the partonic process $ab \to cdV$ is given by $M_{ab,cd}$ and the momentum of the vector boson, appearing in the phase space measure is denoted by $q$.

The real contributions are given by

$$
\left|M^0_{q_i\bar{q}_j, g}\right|^2 = |C_{ij}|^2 \, (v_i^2 + a_i^2)\, N_{1,q\bar{q}}\, A_3^0(\hat{j}_q, 1_g, \hat{i}_{\bar{q}}) \qquad (5.187)
$$

$$
\left|M^0_{q_i g, q_j}\right|^2 = |C_{ij}|^2 \, (v_i^2 + a_i^2)\, N_{1,qg}\, A_3^0(j_q, \hat{1}_g, \hat{i}_{\bar{q}}) \qquad (5.188)
$$

$$
\begin{aligned}
\left|M^0_{q_i\bar{q}_j, gg}\right|^2 &= |C_{ij}|^2 \, (v_i^2 + a_i^2)\, \frac{1}{2} N_{2,q\bar{q}} \Big[N\, A_4^0(\hat{j}_q, 1_g, 2_g, \hat{i}_{\bar{q}}) + N\, A_4^0(\hat{j}_q, 2_g, 1_g, \hat{i}_{\bar{q}}) \\
&\qquad - \frac{1}{N}\, \tilde{A}_4(\hat{j}_q, 1_g, 2_g, \hat{i}_{\bar{q}})\Big]\,, \qquad (5.189)
\end{aligned}
$$

$$
\begin{aligned}
\left|M^0_{q_i\bar{q}_j, q_k\bar{q}_l}\right|^2 &= N_{2,q\bar{q}} \\
\times \Big\{ &\delta_{kl}\, |C_{ij}|^2 \, (v_i^2 + a_i^2)\, B_4^0(\hat{j}_q, k_q, l_{\bar{q}}, \hat{i}_{\bar{q}}) \\
&+ \delta_{ij}\, |C_{kl}|^2 \, (v_k^2 + a_k^2)\, B_4^0(k_q, \hat{j}_q, \hat{i}_{\bar{q}}, l_{\bar{q}}) \\
&+ \delta_{jl}\, |C_{ik}|^2 \, (v_i^2 + a_i^2)\, B_4^0(k_q, \hat{j}_q, l_{\bar{q}}, \hat{i}_{\bar{q}}) \\
&+ \delta_{ik}\, |C_{jl}|^2 \, (v_j^2 + a_j^2)\, B_4^0(\hat{j}_q, k_q, \hat{i}_{\bar{q}}, l_{\bar{q}}) \\
&+ \delta_{ij}\delta_{kl}\, 2\,\Re(C_{ii}C^\dagger_{kk}) \Big(v_i\, v_k\, \hat{B}^0_{4,V}(\hat{j}_q, k_q, l_{\bar{q}}, \hat{i}_{\bar{q}}) + a_i\, a_k\, \hat{B}^0_{4,A}(\hat{j}_q, k_q, l_{\bar{q}}, \hat{i}_{\bar{q}})\Big) \\
&+ \delta_{ik}\delta_{jl}\, 2\,\Re(C_{ii}C^\dagger_{jj}) \Big(v_i\, v_j\, \hat{B}^0_{4,V}(k_q, \hat{j}_q, l_{\bar{q}}, \hat{i}_{\bar{q}}) + a_i\, a_j\, \hat{B}^0_{4,A}(k_q, \hat{j}_q, l_{\bar{q}}, \hat{i}_{\bar{q}})\Big) \\
&+ \frac{2}{N}\, \delta_{ik}\delta_{kl}\, |C_{ij}|^2 \, (v_i^2 + a_i^2)\, C_4^0(\hat{j}_q, k_q, l_{\bar{q}}, \hat{i}_{\bar{q}}) \\
&+ \frac{2}{N}\, \delta_{ij}\delta_{jl}\, |C_{ik}|^2 \, (v_i^2 + a_i^2)\, C_4^0(k_q, \hat{j}_q, l_{\bar{q}}, \hat{i}_{\bar{q}}) \\
&+ \frac{2}{N}\, \delta_{jl}\delta_{kl}\, |C_{ij}|^2 \, (v_i^2 + a_i^2)\, C_4^0(\hat{i}_{\bar{q}}, l_{\bar{q}}, k_q, \hat{j}_q) \\
&+ \frac{2}{N}\, \delta_{ij}\delta_{ik}\, |C_{jk}|^2 \, (v_j^2 + a_j^2)\, C_4^0(l_{\bar{q}}, \hat{i}_{\bar{q}}, k_q, \hat{j}_q)\Big\} \qquad (5.190)
\end{aligned}
$$

$$\begin{aligned}
\left|M^0_{q_iq_j,q_kq_l}\right|^2 &= N_{2,qq}\left(1-\frac{\delta_{kl}}{2}\right)\\
\times\ & \Big\{\delta_{jl}\ |C_{ik}|^2\ (v_i^2+a_i^2)\,B_4^0(k_q,l_q,\hat{j}_{\bar{q}},\hat{i}_{\bar{q}})\\
&+\delta_{ik}\ |C_{jl}|^2\ (v_j^2+a_j^2)\,B_4^0(l_q,k_q,\hat{i}_{\bar{q}},\hat{j}_{\bar{q}})\\
&+\delta_{ik}\delta_{jl}\,2\,\Re(C_{ii}C^\dagger_{jj})\ \Big(v_i\,v_j\,\hat{B}^0_{4,V}(k_q,l_q,\hat{j}_{\bar{q}},\hat{i}_{\bar{q}})+a_i\,a_j\,\hat{B}^0_{4,A}(k_q,l_q,\hat{j}_{\bar{q}},\hat{i}_{\bar{q}})\Big)\Big\}\\
+\ & N_{2,qq}\left(\delta_{ij}\ (1-\delta_{kl})+\frac{\delta_{kl}}{2}\right)\\
\times\ & \Big\{\delta_{jk}\ |C_{il}|^2\ (v_i^2+a_i^2)\,B_4^0(l_q,k_q,\hat{j}_{\bar{q}},\hat{i}_{\bar{q}})\\
&+\delta_{il}\ |C_{jk}|^2\ (v_j^2+a_j^2)\,B_4^0(k_q,l_q,\hat{i}_{\bar{q}},\hat{j}_{\bar{q}})\\
&+\delta_{jk}\delta_{il}\,2\,\Re(C_{ii}C^\dagger_{jj})\ \Big(v_i\,v_j\,\hat{B}^0_{4,V}(l_q,k_q,\hat{j}_{\bar{q}},\hat{i}_{\bar{q}})+a_i\,a_j\,\hat{B}^0_{4,A}(l_q,k_q,\hat{j}_{\bar{q}},\hat{i}_{\bar{q}})\Big)\\
&-\frac{2}{N}\,\delta_{jl}\delta_{jk}\ |C_{ij}|^2\ (v_i^2+a_i^2)\,C_4^0(\hat{i}_{\bar{q}},\hat{j}_{\bar{q}},k_q,l_q)\\
&-\frac{2}{N}\,\delta_{il}\delta_{jl}\ |C_{ik}|^2\ (v_i^2+a_i^2)\,C_4^0(k_q,l_q,\hat{i}_{\bar{q}},\hat{j}_{\bar{q}})\\
&-\frac{2}{N}\,\delta_{ik}\delta_{jk}\ |C_{il}|^2\ (v_i^2+a_i^2)\,C_4^0(l_q,k_q,\hat{i}_{\bar{q}},\hat{j}_{\bar{q}})\\
&-\frac{2}{N}\,\delta_{ik}\delta_{il}\ |C_{ij}|^2\ (v_j^2+a_j^2)\,C_4^0(\hat{j}_{\bar{q}},\hat{i}_{\bar{q}},k_q,l_q)\Big\}\,,
\end{aligned}\tag{5.191}$$

$$\begin{aligned}
\left|M^0_{g_1q_i,g_2q_j}\right|^2 &= |C_{ij}|^2\ (v_i^2+a_i^2)\ N_{2,qg}\Big[N\,A_4^0(j_q,\hat{1}_g,2_g,\hat{i}_{\bar{q}})+N\,A_4^0(j_q,2_g,\hat{1}_g,\hat{i}_{\bar{q}})\\
&\qquad -\frac{1}{N}\,\tilde{A}_4(j_q,\hat{1}_g,2_g,\hat{i}_{\bar{q}})\Big]\,, \qquad (5.192)\\
\left|M^0_{g_1g_2,q_i\bar{q}_j}\right|^2 &= |C_{ij}|^2\ (v_i^2+a_i^2)\,N_{2,gg}\Big[N\,A_4^0(i_q,\hat{1}_g,\hat{2}_g,j_{\bar{q}})+N\,A_4^0(i_q,\hat{2}_g,\hat{1}_g,j_{\bar{q}})\\
&\qquad -\frac{1}{N}\,\tilde{A}_4(i_q,\hat{1}_g,\hat{2}_g,j_{\bar{q}})\Big]\,, \qquad (5.193)
\end{aligned}$$

where

$$\begin{aligned}
N_{n,q\bar{q}} &= N_{n,qq}=4\,\pi\alpha_V\,(g^2)^{n-2}\frac{N^2-1}{N^2}\,(1-\epsilon)\,Q^2\,, && (5.194)\\
N_{n,qg} &= 4\,\pi\alpha_V\,(g^2)^{n-2}\frac{1}{N}\,Q^2\,, && (5.195)\\
N_{n,qg} &= 4\,\pi\alpha_V\,(g^2)^{n-2}\frac{1}{N^2-1}\frac{1}{1-\epsilon}\,Q^2\,, && (5.196)
\end{aligned}$$

with the coupling constants given by

$$\alpha_\gamma=\alpha=\frac{e^2}{4\pi}\,,\qquad \alpha_W=\frac{G_F\,M_W^2\sqrt{2}}{4\pi}\,,\qquad \alpha_Z=\frac{G_F\,M_Z^2\sqrt{2}}{64\pi}\,. \tag{5.197}$$

The vector and axial couplings of the quarks to the vector bosons are

$$
\begin{aligned}
& v_u^\gamma = \frac{2}{3}\,, \qquad v_d^\gamma = -\frac{1}{3}\,, \qquad a_u^\gamma = a_d^\gamma = 0\,, \\
& v_u^Z = 1 - \frac{8}{3}\sin^2\theta_W\,, \qquad v_d^Z = -1 + \frac{4}{3}\sin^2\theta_W\,, \qquad a_u^Z = -1\,, \qquad a_d^Z = 1\,, \\
& v_u^W = v_d^W = \frac{1}{\sqrt{2}}\,, \qquad a_u^W = a_d^W = -\frac{1}{\sqrt{2}}\,.
\end{aligned} \tag{5.198}
$$

The flavor mixing matrices, $C_{ij}$ are given by $\delta_{ij}$ in the case of $\gamma$ and $Z$ production and by the CKM matrix in case of $W$ production. Finally, the colour ordered antenna functions appearing in eqs. (5.188) to (5.194) can be obtained from explicit expressions for the final-final antennae $X_3^0$ and $X_4^0$ in ref. [20] by crossing the particles denoted with hats.

The subtraction terms for this process involve initial-initial and initial-final antennae as there are at most two partons in the final-state, final-final antennae are not needed. Only antennae $A_4^0$ and $B_4^0$ contain singular configurations and, thus, require subtractions. We find the following subtraction terms, classified according to the partonic reaction they must be combined with,

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q_i\bar{q}_j,gg} &= |C_{ij}|^2\,(v_i^2+a_i^2)\,\frac{1}{2}\,N_{2,q\bar{q}}\,\mathrm{d}\Phi_3(k_{g_1},k_{g_2},q;p_q,p_{\bar{q}}) \\
&\times\Big\{N\Big[D^0_{q_i,g_1g_2}\,A^0_{Q_i\bar{q}_j,G}\,J_1^{(1)}(K_G) + D^0_{\bar{q}_j,g_1g_2}\,A^0_{q_i\bar{Q}_j,G}\,J_1^{(1)}(K_G)\Big] \\
&\quad -\frac{1}{N}\Big[A^0_{q_i\bar{q}_j,g_1}\,A^0_{Q_i\bar{Q}_j,G_2}\,J_1^{(1)}(K_{G_2}) + A^0_{q_i\bar{q}_j,g_2}\,A^0_{Q_i\bar{Q}_j,G_1}\,J_1^{(1)}(K_{G_1})\Big]\Big\}\,,
\end{aligned} \tag{5.199}
$$

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q_i\bar{q}_j,q_k\bar{q}_l} &= \sum_{k,l} N_{2,q\bar{q}}\,\mathrm{d}\Phi_3(k_q,k_{\bar{q}},q;p_q,p_{\bar{q}}) \\
&\times\Big\{\delta_{kl}\,|C_{ij}|^2\,(v_i^2+a_i^2)\,\frac{1}{2}\Big(E^0_{q_i,q'_k\bar{q}'_l}\,A^0_{Q_i\bar{q}_j,G}\,J_1^{(1)}(K_G) \\
&\qquad\qquad + E^0_{\bar{q}_j,q'_k\bar{q}'_l}\,A^0_{q_i\bar{Q}_j,G}\,J_1^{(1)}(K_G)\Big) \\
&\quad +\delta_{jl}\,|C_{ik}|^2\,(v_i^2+a_i^2)\,E^0_{\bar{q}_jq'_i,\bar{q}_l}\,A^0_{Q_iG,Q_k}\,J_1^{(1)}(K_{Q_k}) \\
&\quad +\delta_{ik}\,|C_{jl}|^2\,(v_j^2+a_j^2)\,E^0_{q_i\bar{q}'_j,q_k}\,A^0_{\bar{Q}_jG,\bar{Q}_l}\,J_1^{(1)}(K_{Q_l})\Big\}\,,
\end{aligned} \tag{5.200}
$$

(5.201)

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q_iq_j,q_kq_l} &= \sum_{k,l} N_{2,qq}\,\mathrm{d}\Phi_3(k_{q_k},k_{q_l},q;p_{q_i},p_{q_j}) \\
&\times \Bigg\{ \left(1-\frac{\delta_{kl}}{2}\right) \delta_{jl}\,|C_{ik}|^2\,(v_i^2+a_i^2) E^0_{q_j,q_lq_k'}\,A^0_{q_iG,Q_k}\,J_1^{(1)}(K_{Q_k}) \\
&\quad + \left(1-\frac{\delta_{kl}}{2}\right) \delta_{ik}\,|C_{jl}|^2\,(v_j^2+a_j^2) E^0_{q_i,q_kq_l'}\,A^0_{q_jG,Q_l}\,J_1^{(1)}(K_{Q_l}) \\
&+ \left(\delta_{ij}\,(1-\delta_{kl})+\frac{\delta_{kl}}{2}\right) \delta_{jk}\,|C_{il}|^2\,(v_i^2+a_i^2)\,E^0_{q_j,q_kq_l'}\,A^0_{q_iG,Q_l}\,J_1^{(1)}(K_{Q_l}) \\
&+ \left(\delta_{ij}\,(1-\delta_{kl})+\frac{\delta_{kl}}{2}\right) \delta_{il}\,|C_{jk}|^2\,(v_j^2+a_j^2)\,E^0_{q_i,q_lq_k'}\,A^0_{q_jG,Q_k}\,J_1^{(1)}(K_{Q_k}) \Bigg\},
\end{aligned} \tag{5.202}$$

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q_ig,q_jg} &= \sum_j |C_{ij}|^2\,(v_i^2+a_i^2)\,N_{2,qg}\,\mathrm{d}\Phi_3(k_q,k_g,q;p_q,p_g) \\
&\times \Bigg\{ N \Big[ D^0_{q_ig,g}\,A^0_{Q_iG,Q_j}\,J_1^{(1)}(K_{Q_j}) + D^0_{g,gq_j}\,A^0_{q_iG,Q_j}\,J_1^{(1)}(K_{Q_j}) \\
&\qquad + D^0_{g,q_jg}\,A^0_{q_i\bar{Q}_j,G}\,J_1^{(1)}(K_G) \Big] \\
&\quad -\frac{1}{N} \Big[ A^0_{q_i,gq_j}\,A^0_{Q_ig,Q_j}\,J_1^{(1)}(K_{Q_j}) + A^0_{q_ig,q_j}\,A^0_{Q_i\bar{Q}_j,G}\,J_1^{(1)}(K_G) \Big] \Bigg\},
\end{aligned} \tag{5.203}$$

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{g_1g_2,q_i\bar{q}_j} &= \sum_{i,j} |C_{ij}|^2\,(v_i^2+a_i^2)\,N_{2,gg}\,\mathrm{d}\Phi_3(k_q,k_{\bar{q}},q;p_{g_1},p_{g_2}) \\
&\times \frac{N^2-1}{N} \Big[ D^0_{g_1g_2,q_i}\,A^0_{\bar{Q}_iG,\bar{Q}_j}\,J_1^{(1)}(K_{Q_j}) + D^0_{g_1g_2,\bar{q}_j}\,A^0_{Q_jG,Q_i}\,J_1^{(1)}(K_{Q_i}) \Big],
\end{aligned} \tag{5.204}$$

Antennae of the form $X_{iJ,K}$ and $X_{IJ,K}$ correspond to antennae where the momenta of the particles denoted with capital letters are obtained by initial-final and initial-initial phase space mappings respectively.

The integrated form of the subtraction terms can be obtained immediately using the results in Sections 5.4.3 and 5.5.3. The singular pieces of these terms are then given by

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q_i\bar{q}_j,gg} = &\; -2\frac{\alpha_s}{2\pi}\Big[N\,\left(\mathbf{I}^{(1)}_{qg}(t)+\mathbf{I}^{(1)}_{qg}(u)\right) - \frac{1}{N}\,\mathbf{I}^{(1)}_{qq}(s)\Big]\,\mathrm{d}\hat{\sigma}^B_{q_i\bar{q}_j}(p_q,p_{\bar{q}}) \\
&-\frac{\alpha_s}{2\pi}\int\frac{dx}{x}\frac{1}{\epsilon}\,C_F\,p^{(0)}_{qq}(x)\,\left(\mathrm{d}\hat{\sigma}^B_{q_i\bar{q}_j}(x\,p_q,p_{\bar{q}})+\mathrm{d}\hat{\sigma}^B_{q_i\bar{q}_j}(p_q,x\,p_{\bar{q}})\right)+\mathcal{O}(\epsilon^0),
\end{aligned} \tag{5.205}$$

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q_i\bar{q}_j,q_k\bar{q}_l} = &\; -2\frac{\alpha_s}{2\pi}\Big[N_F\,\left(\mathbf{I}^{(1)}_{qg,F}(t)+\mathbf{I}^{(1)}_{qg,F}(u)\right)\Big]\,\mathrm{d}\hat{\sigma}^B_{q_i\bar{q}_j}(p_q,p_{\bar{q}}) \\
&-\frac{\alpha_s}{2\pi}\int\frac{dx}{x}\frac{1}{\epsilon}\,C_F\,p^{(0)}_{gq}(x)\,\left(\mathrm{d}\hat{\sigma}^B_{q_ig}(p_q,x\,p_g)+\mathrm{d}\hat{\sigma}^B_{\bar{q}_jg}(p_{\bar{q}},x\,p_g)\right)+\mathcal{O}(\epsilon^0),
\end{aligned} \tag{5.206}$$

$$
\begin{aligned}
&\mathrm{d}\hat\sigma^{S}_{q_iq_j,q_kq_l} = \\
&\quad -\frac{\alpha_s}{2\pi}\int\frac{dx}{x}\frac{1}{\epsilon}\,C_F\,p^{(0)}_{gq}(x)\,\Big(\mathrm{d}\hat\sigma^{B}_{q_ig}(p_q,x\,p_g)+\mathrm{d}\hat\sigma^{B}_{q_jg}(p_{\bar q},x\,p_g)\Big)+\mathcal{O}(\epsilon^0)\,, \quad (5.207)\\
&\mathrm{d}\hat\sigma^{S}_{q_ig,q_jg} = -2\frac{\alpha_s}{2\pi}\Big[N\,\left(\mathbf{I}^{(1)}_{qg}(u)+\mathbf{I}^{(1)}_{qg}(s)\right)-\frac{1}{N}\,\mathbf{I}^{(1)}_{q\bar q}(t)\\
&\qquad\qquad +N_F\,\Big(\mathbf{I}^{(1)}_{qg,F}(u)+\mathbf{I}^{(1)}_{qg,F}(s)\Big)\Big]\,\mathrm{d}\hat\sigma^{B}_{q_ig}(p_q,p_g)\\
&\quad -\frac{\alpha_s}{2\pi}\int\frac{dx}{x}\frac{1}{\epsilon}\,C_F\,p^{(0)}_{qq}(x)\,\mathrm{d}\hat\sigma^{B}_{q_ig}(x\,p_q,p_g)\\
&\quad -\frac{\alpha_s}{2\pi}\int\frac{dx}{x}\frac{1}{\epsilon}\,\Big(N\,p^{(0)}_{gg}(x)+N\,p^{(0)}_{gg,F}(x)\Big)\,\mathrm{d}\hat\sigma^{B}_{q_ig}(p_q,x\,p_g)\\
&\quad -\frac{\alpha_s}{2\pi}\int\frac{dx}{x}\frac{1}{\epsilon}\,T_F\,p^{(0)}_{qg}(x)\,\sum_j\mathrm{d}\hat\sigma^{B}_{q_i\bar q_j}(p_q,x\,p_{\bar q})+\mathcal{O}(\epsilon^0)\,, \qquad (5.208)\\
&\mathrm{d}\hat\sigma^{S}_{gg,q_i\bar q_j} = \\
&\quad -\frac{\alpha_s}{2\pi}\int\frac{dx}{x}\frac{1}{\epsilon}\,2\,T_F\,p^{(0)}_{qg}(x)\,\sum_i\left(\mathrm{d}\hat\sigma^{B}_{q_ig}(x\,p_q,p_g)+\mathrm{d}\hat\sigma^{B}_{\bar q_ig}(x\,p_{\bar q},p_g)\right)+\mathcal{O}(\epsilon^0)\,,\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (5.209)
\end{aligned}
$$

where the Born cross sections are given by

$$
\begin{aligned}
\mathrm{d}\hat\sigma^{B}_{q_i\bar q_j} &= \mathrm{d}\Phi_2(k_g,q;p_q,p_{\bar q})\,\left|M^0_{q_i\bar q_j,g}\right|^2\,J^{(1)}_1(k_g)\,, && (5.210)\\
\mathrm{d}\hat\sigma^{B}_{q_ig} &= \sum_j\mathrm{d}\Phi_2(k_q,q;p_q,p_g)\,\left|M^0_{q_ig,q_j}\right|^2\,J^{(1)}_1(k_q)\,. && (5.211)
\end{aligned}
$$

Again, the poles in the operators $\mathbf{I}^{(1)}_{ij}$ are canceled by the virtual contributions whereas the ones associated with the Altarelli-Parisi kernels drop out once combined with mass-factorization counterterms.

## 5.8 Conclusions and outlook

In this chapter, we have presented a generalization of the antenna subtraction method for the calculation of higher-order QCD corrections to exclusive collider observables to situations with partons in the initial-state.

The basic ingredients to the subtraction terms, the antenna functions, can be obtained from the known final-state antenna functions by simple crossing. We derived the factorization of an multi-parton phase space into an antenna phase space (required for the analytic integration of the subtraction terms) and a reduced phase space of lower multiplicity,for antennae with one or two hard radiator partons in the initial-state(initial-final and initial-initial antennae). Explicit phase space factorization and parameterization formulae were presented for NLO and NNLO calculations. We derived all integrated initial-final and initial-initial antennae relevant at NLO, and demonstrated their application on two example calculations.

A major advantage of the antenna subtraction method is its straightforward extension to NNLO calculations. The result presented in this chapter are a significant step towards NNLO calculations of hadron collider observables. Using the phase space factorizations presented here, NNLO subtraction terms for jet production observables at hadron colliders can be constructed from known building blocks. Their analytic integration over the antenna phase spaces relevant to NNLO calculations is still an outstanding issue. It is however anticipated that usage of techniques similar to those applied for the integration of the final-final antennae will help to perform these integrals in a systematic and efficient way.

First applications of the method presented here, once the corresponding NNLO integrated antennae are available, could be NNLO calculations of two-jet production or vector-boson-plus-jet production at hadron colliders, and of two-plus-one-jet production in deep inelastic scattering. Further extensions of the method could include radiation off massive particles, thus allowing the NNLO calculation of top quark pair production at hadron colliders.

Another important extension of subtraction methods is the combination with parton shower algorithms [42–44], thus allowing for a full partonic event generation to NLO accuracy. This task has been fully accomplished so far only for one QCD subtraction method [42–44]. While fixed order NLO calculations are independent of the subtraction method used, there can be a residual dependence on the method in matched NLO-plus-parton-shower calculations, since unintegrated and integrated subtraction terms are treated differently in the parton shower. With the formulation of the antenna subtraction method for initial-state radiation presented here, it will become possible to construct antenna-based parton showers for hadronic collisions.

# 5.A One-particle phase space

The one-particle phase space can be expressed through integration over three scalar parameters related to three scalar products.

$$\begin{aligned} s &= 2p_1p_2 && (5.212)\\ \lambda_1 &= \frac{2p_2k}{s} && (5.213)\\ \lambda_2 &= \frac{2p_1k}{s} && (5.214)\\ \lambda_3 &= -\frac{p_Tk}{s} && (5.215)\end{aligned}$$

We work in the center of mass system of $p_1$ and $p_2$, $p_T$ is perpendicular to $p_1, p_2$ and satisfies

$$\vec{k} = \vec{p_1} + \vec{p_2} + \vec{p_T}$$

Due to the symmetry of the problem, only the scattering angle $\Theta$ is relevant. It is given by

$$\sin\Theta = \frac{-p_T \cdot k}{\left|\vec{k}\right|\sqrt{s}}$$

We have

$$\begin{aligned}\int d^dk &= \int dE_k \int d\left|\vec{k}\right| \left|\vec{k}\right|^{d-2}\\ &= V(d-2)\int d(p_1\cdot k)d(p_2\cdot k)d(-p_T\cdot k)\frac{2}{\sqrt{s}^3k}\left|\vec{k}\right|^{d-2}\left(\frac{-p_T\cdot k}{\left|\vec{k}\right|\sqrt{s}}\right)^{d-3}\\ &= \frac{2V(d-2)}{\sqrt{s}^d}\int d(p_1\cdot k)d(p_2\cdot k)d(-p_T\cdot k)(-p_T\cdot k)^{d-3}\\ &= \frac{2V(d-2)}{\sqrt{s}^d}\int \frac{s}{2}d\lambda_1\frac{s}{2}d\lambda_2 s d\lambda_3(s\lambda_3)^{d-3}\\ &= s^{d/2}\frac{V(d-2)}{2}\int d\lambda_1 d\lambda_2 d\lambda_3(\lambda_3)^{d-3} && (5.216)\end{aligned}$$

where

$$V(n) = \frac{2\pi^{n/2}}{\Gamma(n/2)}$$

is the surface of the unit sphere in $n$ dimensions.

# 5.B Expansion in distributions

The integration of the antenna functions for the initial-initial case are trivial, since the integration over the phase-space of the unresolved particle in (5.49)

$$\int [\mathrm{d}k] x_1 x_2 \delta(x_1 - \hat{x}_1)\delta(x_2 - \hat{x}_2) \tag{5.217}$$

is, up to a trivial angle integration, frozen by the two $\delta$-functions. This section explains how to express the "integrated" antenna functions in terms of distributions.

We first use the phase-space parameterization of the preceding section 5.A

$$\int d^d k \quad = \quad s^{d/2} \frac{V(d-2)}{2} \int d\lambda_1 d\lambda_2 d\lambda_3 (\lambda_3)^{d-3} \,. \tag{5.218}$$

In terms of the $\lambda$ variables we have

$$\begin{aligned} k^2 &= s\left(\lambda_1\lambda_2 - \lambda_3^2\right) \\ \hat{x}_1 &= \sqrt{\frac{(1-\lambda_1)(1-\lambda_1-\lambda_2)}{1-\lambda_2}} \\ \hat{x}_2 &= \sqrt{\frac{(1-\lambda_2)(1-\lambda_1-\lambda_2)}{1-\lambda_1}} \,, \end{aligned} \tag{5.219}$$

so that (5.218) becomes

$$\begin{aligned} &\int [\mathrm{d}k] x_1 x_2 \delta(x_1 - \hat{x}_1)\delta(x_2 - \hat{x}_2) \\ &= \frac{1}{(2\pi)^{d-1}} \int \mathrm{d}^d k \delta(k^2) x_1 x_2 \delta(x_1 - \hat{x}_1)\delta(x_2 - \hat{x}_2) \\ &= s_{12}^{d/2} \frac{V(d-2)}{2(2\pi)^{d-1}} d\lambda_1 d\lambda_2 d\lambda_3 (\lambda_3)^{d-3} \delta(\lambda_1\lambda_2 - \lambda_3^2) x_1 x_2 \\ &\quad \times \delta\left(x_1 - \sqrt{\frac{(1-\lambda_1)(1-\lambda_1-\lambda_2)}{1-\lambda_2}}\right) \delta\left(x_2 - \sqrt{\frac{(1-\lambda_2)(1-\lambda_1-\lambda_2)}{1-\lambda_1}}\right) \\ &= s_{12}^{1-\epsilon} \frac{2(4\pi)^{-\frac{d}{2}}}{\Gamma(1-\epsilon)} \left(\frac{x_1 x_2 (1+x_1)(1+x_2)}{(x_1+x_2)^2}\right)^{\epsilon} \\ &\quad \times (1-x_1)^{-1-\epsilon}(1-x_2)^{-1-\epsilon} \left(\frac{x_1^2 x_2^2 (1+x_1 x_2)}{(x_1+x_2)^2}\right) \\ &= Q^{1-\epsilon} \frac{2(4\pi)^{-\frac{d}{2}}}{\Gamma(1-\epsilon)} \mathcal{J}(x_1, x_2) \,, \end{aligned} \tag{5.220}$$

with $Q^2 = (p_1 + p_2 - p_k)^2 = x_1 x_2 s_{12}$. The Jacobian given as in equation (5.51) by

$$\mathcal{J}(x_1, x_2) = \frac{x_1\, x_2\, (1 + x_1\, x_2)}{(x_1 + x_2)^2}\, (1 - x_1)^{-\epsilon} (1 - x_2)^{-\epsilon} \left( \frac{(1 + x_1)(1 + x_2)}{(x_1 + x_2)^2} \right)^{-\epsilon} , \tag{5.221}$$

and the two-particle invariants are as in (5.52)

$$s_{1j} = -s_{12} \frac{x_1\,(1 - x_2^2)}{x_1 + x_2} , \qquad s_{j2} = -s_{12} \frac{x_2\,(1 - x_1^2)}{x_1 + x_2} . \tag{5.222}$$

The expansion in distributions is done by using the following identities.

$$\begin{aligned}
&\int_0^1 \frac{\phi(x)}{(1-x)^{1+\epsilon}} \mathrm{d}x \\
&= \int_0^1 \frac{\phi(x) - \phi(1)}{(1-x)^{1+\epsilon}} \mathrm{d}x + \phi(1) \int_0^1 \frac{\mathrm{d}x}{(1-x)^{1+\epsilon}} \\
&= \int_0^1 (\phi(x) - \phi(1)) \sum_{n=0}^{\infty} \frac{(-\epsilon)^n \log^n(1-x)}{(1-x) n!} \mathrm{d}x + \phi(1)\, \frac{1}{\epsilon} (1-x)^{\epsilon} \Big|_0^1 \\
&= \int_0^1 (\phi(x) - \phi(1)) \sum_{n=0}^{\infty} \frac{(-\epsilon)^n \log^n(1-x)}{(1-x) n!} \mathrm{d}x - \phi(1) \frac{1}{\epsilon} \\
&= \int_0^1 \left[ -\frac{1}{\epsilon} \delta(1-x) + \sum_{n=0}^{\infty} \frac{(-\epsilon)^n}{n!} \left( \frac{\log^n(1-x)}{1-x} \right)_+ \right] \phi(x) \mathrm{d}x \\
&= \int_0^1 \left[ -\frac{1}{\epsilon} \delta(1-x) + \left( \frac{1}{1-x} \right)_+ - \epsilon \left( \frac{\log(1-x)}{1-x} \right)_+ + \mathcal{O}(\epsilon^2) \right] \phi(x) \mathrm{d}x ,
\end{aligned} \tag{5.223}$$

where the $\epsilon$ expansion in the second line can be performed, because the integrand is finite. We made use of the definition of the plus distribution

$$\int dx\, (f(x))_+\, \phi(x) = \int dx f(x)\, (\phi(x) - \phi(1)) \ . \tag{5.224}$$

For $n \geq 0$ we have

$$\begin{aligned}\int_0^1 (1-x)^{n-\epsilon}\phi(x)\mathrm{d}x &= \int_0^1 (1-x)^n \sum_{j=0}^{\infty} \frac{(-\epsilon)^j \log^j(1-x)}{j!}\,\phi(x)\mathrm{d}x \\ &= \sum_{j=0}^{\infty} \frac{(-\epsilon)^j}{j!} \int_0^1 (1-x)^n \log^j(1-x)\,\phi(x)\mathrm{d}x\;,\end{aligned} \tag{5.225}$$

where we could expand the rhs of the first line, since for positive $n$ the integrand is finite.

We illustrate the expansion of the initial-initial antenna function in distribution with the example function

$$f(s_{12}, s_{1j}, s_{j2}) = \frac{\Gamma(1-\epsilon)(4\pi)^{2-\epsilon}}{2Q^{1-\epsilon}} \frac{s_{12}^2}{s_{1j}s_{j2}}\;.$$

We compute

$$\begin{aligned} I \equiv \int dx_1 dx_2 &\int [dk] x_1 x_2 \delta(x_1 - \hat{x}_1)\delta(x_2 - \hat{x}_2) f(s_{12}, s_{1j}, s_{j2})\;\phi(x_1, x_2) \\ = &\int dx_1 dx_2 \mathcal{J}(x_1, x_2) \frac{(x_1 + x_2)^2}{x_1\,(1 - x_2^2) x_2\,(1 - x_1^2)}\;\phi(x_1, x_2) \\ = &\int dx_1 dx_2 \frac{(1 + x_1\,x_2)}{(1 + x_2)\,(1 + x_1)}\;(1 - x_1)^{-1-\epsilon}(1 - x_2)^{-1-\epsilon} \\ &\times \left(\frac{(1 + x_1)(1 + x_2)}{(x_1 + x_2)^2}\right)^{-\epsilon} \phi(x_1, x_2)\;. \end{aligned} \tag{5.226}$$

The factors $(1-x)^{-1-\epsilon}$ will give rise to the poles in $\epsilon$. We will only consider the expansion in $\epsilon$ up to the finite terms, so we can expand the last factor of (5.227) and drop the terms of higher order than $\epsilon^2$. We use partial fractioning to disentangle the factors $(1 - x_i)$ in the denominator,

$$\begin{aligned} I \;=\; &\int dx_1 dx_2 (1 - x_1)^{-\epsilon}(1 - x_2)^{-\epsilon} \left(\frac{1}{2(1 + x_2)\,(1 + x_1)} + \frac{1}{2(1 - x_1)(1 - x_2)}\right) \\ &\times \left(1 - \epsilon \log\left(\frac{(1 + x_1)(1 + x_2)}{(x_1 + x_2)^2}\right) + \frac{1}{2}\epsilon^2 \log^2\left(\frac{(1 + x_1)(1 + x_2)}{(x_1 + x_2)^2}\right) + \mathcal{O}(\epsilon^3)\right) \\ &\times \phi(x_1, x_2)\;. \end{aligned} \tag{5.227}$$

The first term is finite when we expand in $\epsilon$. For the second term, we use 5.224 and get

$$
\begin{aligned}
I = &+\frac{1}{2}\int dx_1 dx_2 \frac{\phi(x_1,x_2)}{(1+x_2)\,(1+x_1)} \\
+ &\ \frac{1}{2}\int dx_1 dx_2 \left(-\frac{1}{\epsilon}\delta(1-x_1) + \left(\frac{1}{1-x_1}\right)_+ - \epsilon\left(\frac{\log(1-x_1)}{1-x_1}\right)_+\right) \\
&\times \left(-\frac{1}{\epsilon}\delta(1-x_2) + \left(\frac{1}{1-x_2}\right)_+ - \epsilon\left(\frac{\log(1-x_2)}{1-x_2}\right)_+\right) \\
&\times \left(1 - \epsilon\log\left(\frac{(1+x_1)(1+x_2)}{(x_1+x_2)^2}\right) + \frac{1}{2}\epsilon^2\log^2\left(\frac{(1+x_1)(1+x_2)}{(x_1+x_2)^2}\right) + \mathcal{O}(\epsilon^3)\right) \\
&\times\phi(x_1,x_2) \\
.
\end{aligned}
\tag{5.228}
$$

Using the "commutation" relations

$$
\begin{aligned}
\int dx \left(\frac{1}{1-x}\right)_+ f(x)\phi(x) &= \int dx \frac{f(x)\phi(x) - f(1)\phi(1)}{1-x} \\
&= \int dx \frac{f(x)\phi(x) - f(1)\phi(x) + f(1)\phi(x) - f(1)\phi(1)}{1-x} \\
&= \int dx \frac{f(x)-f(1)}{1-x}\phi(x) + f(1)\frac{\phi(x)-\phi(1)}{1-x} \\
&= \int dx \left[\frac{f(x)-f(1)}{1-x} + f(1)\left(\frac{1}{1-x}\right)_+\right]\phi(x)
\end{aligned}
\tag{5.229}
$$

$$
\int dx\delta(1-x)f(x)\phi(x) = \int dx f(1)\phi(1) = \int dx f(1)\left[\delta(1-x)\right]\phi(x)\ , \tag{5.230}
$$

we finally get

$$
\begin{aligned}
I \ = \ \frac{1}{2}\int dx_1 dx_2 \Bigg[ &\frac{1}{\epsilon^2}\delta(1-x_1)\delta(1-x_2) \\
&-\frac{1}{\epsilon}\left(\delta(1-x_1)\left(\frac{1}{1-x_2}\right)_+ + \delta(1-x_2)\left(\frac{1}{1-x_1}\right)_+\right) \\
&+\delta(1-x_1)\left(\log\frac{2}{1+x_2} + \left(\frac{\log(1-x_2)}{1-x_2}\right)_+\right) \\
&+\delta(1-x_2)\left(\log\frac{2}{1+x_1} + \left(\frac{\log(1-x_1)}{1-x_1}\right)_+\right) \\
&+\left(\frac{1}{1-x_1}\right)_+\left(\frac{1}{1-x_2}\right)_+ + \frac{1}{(1+x_1)(1+x_2)}\Bigg]\phi(x_1,x_2)\ .
\end{aligned}
\tag{5.231}
$$

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# Part II

# Applications

# Chapter 6

# Master integrals

*This chapter is based on the paper*

*"Two-Loop Quark and Gluon Form Factors"*

*published with Tobias Huber and Thomas Gehrmann in Physics Letters B [1].*

## 6.1 Introduction

The infrared pole structure of renormalized multi-loop amplitudes in dimensional regularization with $d = 4 - 2\epsilon$ space-time dimensions can be predicted from an infrared factorization formula, which was first conjectured in ref. [2], where it was formulated up to two loops. A proof of the formula, together with an explicit formulation up to three loops was derived later in ref. [3]. The simplest multi-loop amplitudes where the infrared factorization formula can be applied are three-point functions, involving two partons coupled to an external current: the quark form factor $\gamma^* \to q\bar{q}$ and the gluon form factor $H \to gg$. The QCD corrections to these form factors can in particular be used to fix a priori unknown constants in the infrared factorization formula, thus enabling an unambiguous prediction for multi-loop amplitudes involving more than two external partons.

In the infrared factorization formula for a given form factor (or more generally for a given multi-leg amplitude) at a certain number of loops, infrared singularity operators act on the form factor evaluated with a lower number of loops. The infrared singularity operators contain explicit infrared poles $1/\epsilon^2$ and $1/\epsilon$. They do therefore project subleading terms in $\epsilon$ from the lower order form factors.

At present, two-loop corrections to the massless quark [4–6] and gluon [7] form factors are known to order $\epsilon^0$. Two-loop corrections to this order were also obtained for massive quarks [8–10]. The infrared structure of the massless form factors and infrared cancellations with real radiation contributions are described in detail in ref. [11–14]. Very recently, results to order $\epsilon^2$ were obtained for the quark form factor [15].

The calculation of these corrections proceeds through a reduction [16–20] of all two-loop Feynman integrals appearing in the form factors to a small set of master integrals. The reduction is exact in $\epsilon$, so that the evaluation of the form factors is limited only by the order to which the master integrals can be computed. The massless two-loop form factors contain three two-loop master integrals, which can be computed either using various analytical methods [21] or numerically order-by-order in their Laurent expansion using the sector decomposition algorithm [22, 23]. Up to now, exact expressions were known only for two of these master integrals, while the third (the so-called two-loop crossed triangle graph) was known only as a Laurent expansion up to finite terms [24–26].

In this section, we derive an exact expression for the two-loop crossed triangle graph in terms of generalized hypergeometric functions of unit argument in section 6.2. Using the `HypExp`-package described in chapter 3 for the Laurent expansion of generalized hypergeometric functions, this can be expanded to any desired order in $\epsilon$. Together with the exact expressions for the one- and two-loop quark and gluon form factors in Section 6.2.1, this allows the expansion of these form factors to higher orders in $\epsilon$. For illustration, we list the one-loop form factors to order $\epsilon^4$ and the two-loop form factors to order $\epsilon^2$ in Section 6.2.2; these orders appear for example in the infrared factorization of the corresponding three-loop form factors.

## 6.2 Two-loop master integrals

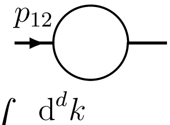
The virtual two-loop vertex master integrals were first derived to order $\epsilon^0$ in refs. [24–26] in the context of the calculation of the two-loop quark form factor [4–6]. All but the crossed triangle graph $A_6$ can be expressed in terms of $\Gamma$-functions to all orders in $\epsilon$.

Factoring out a common factor,

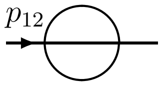
$$S_\Gamma = \left(\frac{(4\pi)^\epsilon}{16\pi^2\,\Gamma(1-\epsilon)}\right) , \tag{6.1}$$

and introducing $q^2 = (p_1+p_2)^2$, they read

$$A_{2,\mathrm{LO}} =$$

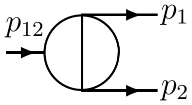



$$\begin{aligned} &= \int \frac{\mathrm{d}^d k}{(2\pi)^d}\,\frac{1}{k^2(k-p_1-p_2)^2} \\ &= S_\Gamma\,\left(-q^2\right)^{-\epsilon}\,\frac{\Gamma(1+\epsilon)\Gamma^3(1-\epsilon)}{\Gamma(2-2\epsilon)}\,\frac{i}{\epsilon}\,, \end{aligned} \tag{6.2}$$

$A_3 =$ 

$$= \int \frac{\mathrm{d}^d k}{(2\pi)^d} \int \frac{\mathrm{d}^d l}{(2\pi)^d} \frac{1}{k^2 l^2 (k-l-p_1-p_2)^2}$$

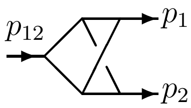
$$= S_\Gamma^2 \left(-q^2\right)^{1-2\epsilon} \frac{\Gamma(1+2\epsilon)\Gamma^5(1-\epsilon)}{\Gamma(3-3\epsilon)} \frac{-1}{2(1-2\epsilon)\epsilon} \,, \tag{6.3}$$

$A_4 =$ 

$$= \int \frac{\mathrm{d}^d k}{(2\pi)^d} \int \frac{\mathrm{d}^d l}{(2\pi)^d} \frac{1}{k^2 l^2 (k-p_1-p_2)^2 (k-l-p_1)^2}$$

$$= S_\Gamma^2 \left(-q^2\right)^{-2\epsilon} \frac{\Gamma(1-2\epsilon)\Gamma(1+\epsilon)\Gamma^4(1-\epsilon)\Gamma(1+2\epsilon)}{\Gamma(2-3\epsilon)} \frac{-1}{2(1-2\epsilon)\epsilon^2} \,. \tag{6.4}$$

No exact expression for $A_6$ was known up to now. Following the steps outlined in refs. [4–6], we obtain

$A_6 =$ 

$$= \int \frac{\mathrm{d}^d k}{(2\pi)^d} \int \frac{\mathrm{d}^d l}{(2\pi)^d} \frac{1}{k^2 l^2 (k-p_1-p_2)^2 (k-l)^2 (k-l-p_2)^2 (l-p_1)^2}$$

$$\begin{aligned} = {} & S_\Gamma^2 \left(-q^2\right)^{-2-2\epsilon} \Bigg[ -\frac{\Gamma^3(1-\epsilon)\,\Gamma(1+\epsilon)\,\Gamma^4(1-2\epsilon)\,\Gamma^3(1+2\epsilon)}{\epsilon^4\,\Gamma^2(1-4\epsilon)\,\Gamma(1+4\epsilon)} \\ & + \frac{\Gamma^4(1-\epsilon)\,\Gamma(1+\epsilon)\,\Gamma(1-2\epsilon)\,\Gamma(1+2\epsilon)}{2\,\epsilon^4\,\Gamma(1-3\epsilon)} \,{}_3F_2(1,-4\epsilon,-2\epsilon;1-3\epsilon,1-2\epsilon;1) \\ & - \frac{4\,\Gamma^4(1-\epsilon)\,\Gamma(1-2\epsilon)\,\Gamma(1+2\epsilon)}{\epsilon^2\,(1+\epsilon)\,(1+2\epsilon)\,\Gamma(1-4\epsilon)} \,{}_3F_2(1,1,1+2\epsilon;2+\epsilon,2+2\epsilon;1) \\ & - \frac{\Gamma^5(1-\epsilon)\,\Gamma(1+2\epsilon)}{2\,\epsilon^4\,\Gamma(1-3\epsilon)} \,{}_4F_3(1,1-\epsilon,-4\epsilon,-2\epsilon;1-3\epsilon,1-2\epsilon,1-2\epsilon;1) \Bigg] \,. \end{aligned} \tag{6.5}$$

While $A_{2,LO}$, $A_3$ and $A_4$ can be expanded using any standard computer algebra program, the expansion of $A_6$ requires the expansion of generalized hypergeometric functions in their parameters. For this task we can use the package `HypExp` presented in chapter 3. The expansion of the master integrals reads

$$
\begin{aligned}
A_3 &= S_\Gamma \left(-q^2\right)^{1-2\epsilon} \Bigg[ -\frac{1}{4\epsilon} - \frac{13}{8} - \frac{115}{16}\,\epsilon + \left(-\frac{865}{32} + \frac{5}{2}\zeta_3\right)\epsilon^2 \\
&\quad + \left(-\frac{5971}{64} + \frac{65}{4}\zeta_3 + \frac{\pi^4}{24}\right)\epsilon^3 + \left(\frac{575}{8}\zeta_3 + \frac{13\pi^4}{48} + \frac{27}{2}\zeta_5 - \frac{39193}{128}\right)\epsilon^4 \\
&\quad + \left(\frac{4325}{16}\zeta_3 + \frac{115\pi^4}{96} + \frac{351}{4}\zeta_5 + \frac{11\pi^6}{378} - \frac{25}{2}\zeta_3^2 - \frac{249355}{256}\right)\epsilon^5 + \mathcal{O}(\epsilon^6)\Bigg] ,
\end{aligned}
\tag{6.6}
$$

$$
\begin{aligned}
A_4 &= S_\Gamma \left(-q^2\right)^{1-2\epsilon} \Bigg[ -\frac{1}{2\epsilon^2} - \frac{5}{2\epsilon} + \left(-\frac{\pi^2}{6} - \frac{19}{2}\right) + \left(4\zeta_3 - \frac{5\pi^2}{6} - \frac{65}{2}\right)\epsilon \\
&\quad + \left(-\frac{19\pi^2}{6} + 20\zeta_3 + \frac{\pi^4}{30} - \frac{211}{2}\right)\epsilon^2 \\
&\quad + \left(-\frac{65\pi^2}{6} + \frac{4\pi^2}{3}\zeta_3 + 76\zeta_3 + \frac{\pi^4}{6} + 24\zeta_5 - \frac{665}{2}\right)\epsilon^3 \\
&\quad + \Bigg( -\frac{211\pi^2}{6} + \frac{20\pi^2}{3}\zeta_3 + 260\zeta(3) + \frac{19\pi^4}{30} + 120\zeta_5 \\
&\qquad + \frac{22\pi^6}{315} - 16\zeta_3^2 - \frac{2059}{2}\Bigg)\epsilon^4 + \mathcal{O}(\epsilon^5)\Bigg] ,
\end{aligned}
\tag{6.7}
$$

$$
\begin{aligned}
A_6 &= S_\Gamma^2 \left(-q^2\right)^{-2-2\epsilon} \Bigg[ -\frac{1}{\epsilon^4} + \frac{5\pi^2}{6\epsilon^2} + \frac{27}{\epsilon}\zeta_3 + \frac{23\pi^4}{36} + \left(117\zeta_5 - 8\pi^2\zeta_3\right)\epsilon \\
&\quad + \left(\frac{19\pi^6}{315} - 267\zeta_3^2\right)\epsilon^2 + \left(-\frac{109\pi^4}{10}\zeta_3 - 40\pi^2\zeta_5 - 6\zeta_7\right)\epsilon^3 \\
&\quad + \left(44\pi^2\zeta_3^2 - \frac{1073\pi^8}{3024} - 2466\,\zeta_3\,\zeta_5 + 264\zeta_{5,3}\right)\epsilon^4 + \mathcal{O}(\epsilon^5)\Bigg] ,
\end{aligned}
\tag{6.8}
$$

where we encountered a multiple zeta value in the last term.

### 6.2.1 Quark and gluon form factors at two loops

The tree-level quark and gluon form factors are obtained by normalizing the corresponding tree-level vertex functions to unity:

$$F_q^{(0l)} = 1\,, \qquad F_g^{(0l)} = 1\,. \tag{6.9}$$

The unrenormalized one-loop and two-loop form factors are calculated from the relevant Feynman diagrams. Using integration-by-parts [16, 17] and Lorentz invariance [19] identities (which can be solved symbolically for massless two-loop vertex integrals, see the appendix of ref. [27]), these can be reduced [18–20] to the master integrals listed in Section 6.2.

The unrenormalized one-loop quark and gluon form factors read:

$$F_q^{(1l,B)} = -ig^2\,\frac{N^2-1}{N}\,\frac{d^2-7d+16}{2\,(d-4)}\,A_{2,\mathrm{LO}}\,, \tag{6.10}$$

$$F_g^{(1l,B)} = ig^2\,N\,\frac{d^3-16d^2+68d-88}{(d-4)\,(d-2)}\,A_{2,\mathrm{LO}}\,, \tag{6.11}$$

where $N=3$ is the number of colours and $g$ is the bare QCD coupling parameter.

The unrenormalized two-loop quark and gluon form factors for $N_F$ massless quark flavors are:

$$\begin{aligned}
F_q^{(2l,B)} = g^4\,\frac{N^2-1}{N}\Bigg\{ &-\frac{N^2-1}{N}\,\frac{(d^2-7d+16)^2}{4\,(d-4)^2}\,A_{2,\mathrm{LO}}^2 \\
&+N\,\frac{(d^5-18d^4+138d^3-552d^2+1144d-980)\,(3d-8)}{2\,(d-3)\,(d-4)^3}\,\frac{A_3}{q^2} \\
&+\frac{1}{N}\,(9d^6-358d^5+4309d^4-24466d^3+72896d^2-110064d+66080) \\
&\qquad\times\frac{(3d-8)}{16(d-3)(d-4)^3(2d-7)}\,\frac{A_3}{q^2} \\
&+N\,\frac{3d^6-82d^5+819d^4-4030d^3+10344d^2-12824d+5632}{4\,(d-1)\,(d-4)^2\,(3d-8)}\,A_4 \\
&-\frac{1}{N}\,\frac{(21d^6-789d^5+9422d^4-53864d^3+163200d^2-253472d+159232)}{16\,(3d-8)\,(2d-7)\,(d-4)^2}\,A_4 \\
&+N_F\,\frac{(3d^3-31d^2+110d-128)\,(d-2)}{2\,(d-1)\,(d-4)\,(3d-8)}\,A_4 \\
&-\frac{1}{N}\,\frac{d^3-20d^2+104d-176}{32\,(2d-7)}(q^2)^2\,A_6\Bigg\}\,,
\end{aligned} \tag{6.12}$$

$$
\begin{aligned}
F_g^{(2l,B)} = g^4 \Bigg\{ & - N^2 \frac{(d^3-16d^2+68d-88)^2}{(d-4)^2\,(d-2)^2}\, A^2_{2,\mathrm{LO}} \\
& -N^2 \frac{1}{2\,(d-1)\,(d-2)^2\,(d-3)\,(d-4)^3\,(2d-5)\,(2d-7)} \Big(192d^{10}-6947d^9 \\
& \quad +105470d^8-907248d^7+4958664d^6-18113645d^5+44930982d^4 \\
& \quad -74791460d^3+79854504d^2-49204128d+13194496\Big)\frac{A_3}{q^2} \\
& -N\,N_F \frac{2d^6-45d^5+377d^4-1610d^3+3868d^2-5136d+3008}{(d-1)\,(d-2)\,(d-3)\,(d-4)^2}\frac{A_3}{q^2} \\
& +\frac{N_F}{N}\frac{1}{4\,(d-2)\,(d-3)\,(d-4)^2\,(2d-5)\,(2d-7)}\Big(70d^7-1663d^6+16290d^5 \\
& \quad -86031d^4+266004d^3-483356d^2+479360d-200704\Big)\frac{A_3}{q^2} \\
& -N^2 \frac{1}{2\,(d-1)\,(d-2)^2\,(d-4)^2\,(2d-5)\,(2d-7)} \\
& \Big(108d^8-2661d^7+28822d^6-177546d^5+674735d^4 \\
& \quad -1607602d^3+2325996d^2-1848920d+607968\Big)A_4 \\
& +N\,N_F \frac{2d^4-28d^3+130d^2-228d+104}{(d-1)\,(d-2)\,(d-4)} A_4 \\
& -\frac{N_F}{N}\frac{(46d^4-545d^3+2395d^2-4606d+3248)\,(d-6)}{4\,(d-2)\,(d-4)\,(2d-5)\,(2d-7)} A_4 \\
& -N^2 \frac{3\,(3d-8)\,(d-3)}{4\,(2d-5)\,(2d-7)}(q^2)^2 A_6 \\
& -\frac{N_F}{N}\frac{(d-4)\,(2d^3-25d^2+94d-112)}{8\,(d-2)\,(2d-5)\,(2d-7)}(q^2)^2 A_6 \Bigg\} . 
\end{aligned} \tag{6.13}
$$

The renormalized form factors are obtained by introducing the renormalized QCD coupling constant and the renormalized effective coupling of $H$ to the gluon field strength [7], and subsequent expansion in powers of the renormalized coupling.

### 6.2.2 Expansion of two-loop form factors

The renormalized form factors are expanded in the renormalized coupling constant. In the $\overline{\mathrm{MS}}$ scheme, the bare coupling $\alpha_0 = g^2/(4\pi)$ is related to the renormalized coupling $\alpha_s \equiv \alpha_s(\mu^2)$, evaluated at the renormalization scale $\mu^2$ by

$$
\alpha_0 \mu_0^{2\epsilon} S_\epsilon = \alpha_s \mu^{2\epsilon}\left[1 - \frac{11N-2N_F}{6\epsilon}\left(\frac{\alpha_s}{2\pi}\right) + \mathcal{O}(\alpha_s^2)\right] , \tag{6.14}
$$

where

$$
S_\epsilon = (4\pi)^\epsilon e^{-\epsilon\gamma} \qquad \text{with the Euler constant } \gamma = 0.5772\ldots
$$

and $\mu_0^2$ is the mass parameter introduced in dimensional regularization to maintain a dimensionless coupling in the bare QCD Lagrangian density. For simplicity, we set $\mu^2 = q^2$. If the squared momentum transfer $q^2$ is space-like ($q^2 < 0$), the form factors are real, while they acquire imaginary parts for time-like $q^2$. These imaginary parts (and corresponding real parts) arise from the $\epsilon$-expansion of

$$\Delta(q^2) = (-\mathrm{sgn}(q^2) - i0)^{-\epsilon} \ . \tag{6.15}$$

The renormalized form factors can then be written as

$$F_{q,g}(q^2) = 1 + \left(\frac{\alpha_s}{2\pi}\,\Delta(q^2)\right) F_{q,g}^{(1)} + \left(\frac{\alpha_s}{2\pi}\,\Delta(q^2)\right)^2 F_{q,g}^{(2)} + \mathcal{O}(\alpha_s^3) \ . \tag{6.16}$$

Expanding the first and second order coefficients of the form factors to $\epsilon^4$ and $\epsilon^2$ respectively, we obtain:

$$\begin{aligned} F_q^{(1)} &= \left(N - \frac{1}{N}\right)\Bigg[-\frac{1}{2\epsilon^2} - \frac{3}{4\epsilon} - 2 + \frac{\pi^2}{24} + \left(-4 + \frac{\pi^2}{16} + \frac{7}{6}\zeta_3\right)\epsilon \\ &\quad + \left(-8 + \frac{\pi^2}{6} + \frac{7}{4}\zeta_3 - \frac{47\pi^4}{2880}\right)\epsilon^2 \\ &\quad + \left(-16 - \frac{7\pi^2}{72}\zeta_3 + \frac{14}{3}\zeta_3 + \frac{31}{10}\zeta_5 + \frac{\pi^2}{3} + \frac{47\pi^4}{1920}\right)\epsilon^3 \\ &\quad + \left(-32 - \frac{7\pi^2}{48}\zeta_3 + \frac{28}{3}\zeta_3 - \frac{49}{36}\zeta_3^2 + \frac{93}{20}\zeta_5 + \frac{2\pi^2}{3} + \frac{47\pi^4}{720} + \frac{949\pi^6}{241920}\right)\epsilon^4\Bigg] \\ &\quad + \mathcal{O}(\epsilon^5) \ , \end{aligned} \tag{6.17}$$

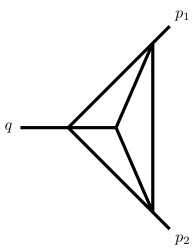
$$\begin{aligned} F_g^{(1)} &= N\Bigg[-\frac{1}{\epsilon^2} - \frac{11}{6\epsilon} + \frac{\pi^2}{12} + \left(-1 + \frac{7}{3}\zeta_3\right)\epsilon + \left(-3 + \frac{47\pi^4}{1440}\right)\epsilon^2 \\ &\quad + \left(-7 - \frac{7\pi^2}{36}\zeta_3 + \frac{31}{5}\zeta_5 + \frac{\pi^2}{12}\right)\epsilon^3 \\ &\quad + \left(-15 + \frac{7}{3}\zeta_3 - \frac{49}{18}\zeta_3^2 + \frac{\pi^2}{4} + \frac{949\pi^6}{120960}\right)\epsilon^4\Bigg] + \frac{N_F}{3\epsilon} + \mathcal{O}(\epsilon^5), \end{aligned} \tag{6.18}$$

$$
\begin{aligned}
F_q^{(2)} &= \left(N-\frac{1}{N}\right)\ \Bigg\{ N\Bigg[\frac{1}{8\epsilon^4}+\frac{17}{16\epsilon^3}+\frac{433}{288\epsilon^2} \\
&+\frac{1}{\epsilon}\left(\frac{4045}{1728}-\frac{11\pi^2}{96}+\frac{7}{24}\zeta_3\right) \\
&+\left(-\frac{9083}{10368}-\frac{521\pi^2}{1728}+\frac{13}{18}\zeta_3+\frac{23\pi^4}{2880}\right) \\
&+\left(-\frac{1244339}{62208}-\frac{11\pi^2}{48}\zeta_3+\frac{4235}{432}\zeta_3+\frac{163}{40}\zeta_5-\frac{10427\pi^2}{10368}+\frac{29\pi^4}{1440}\right)\epsilon \\
&+\Bigg(-\frac{36528395}{373248}-\frac{77\pi^2}{432}\zeta_3+\frac{109019}{2592}\zeta_3-\frac{403}{72}\zeta_3^2+\frac{529}{30}\zeta_5 \\
&\qquad -\frac{181451\pi^2}{62208}+\frac{8759\pi^4}{51840}+\frac{47\pi^6}{7560}\Bigg)\epsilon^2\Bigg] \\
&+\frac{1}{N}\Bigg[-\frac{1}{8\epsilon^4}-\frac{3}{8\epsilon^3}+\frac{1}{\epsilon^2}\left(-\frac{41}{32}+\frac{\pi^2}{48}\right) \\
&+\frac{1}{\epsilon}\left(-\frac{221}{64}+\frac{4}{3}\zeta_3\right) \\
&+\left(-\frac{1151}{128}-\frac{17\pi^2}{192}+\frac{29}{8}\zeta_3+\frac{13\pi^4}{576}\right) \\
&+\left(-\frac{5741}{256}-\frac{7\pi^2}{18}\zeta_3+\frac{839}{48}\zeta_3+\frac{23}{10}\zeta_5-\frac{71\pi^2}{128}+\frac{19\pi^4}{320}\right)\epsilon \\
&+\Bigg(-\frac{27911}{512}-\frac{9\pi^2}{16}\zeta_3+\frac{6989}{96}\zeta_3-\frac{163}{9}\zeta_3^2 \\
&\qquad +\frac{231}{40}\zeta_5-\frac{613\pi^2}{256}+\frac{3401\pi^4}{11520}-\frac{223\pi^6}{17280}\Bigg)\epsilon^2\Bigg] \\
&+N_F\Bigg[-\frac{1}{8\epsilon^3}-\frac{1}{18\epsilon^2}+\frac{1}{\epsilon}\left(\frac{65}{432}+\frac{\pi^2}{48}\right) \\
&+\left(\frac{4085}{2592}+\frac{23\pi^2}{432}+\frac{1}{36}\zeta_3\right) \\
&+\left(\frac{108653}{15552}-\frac{119}{108}\zeta_3+\frac{497\pi^2}{2592}+\frac{\pi^4}{1440}\right)\epsilon \\
&+\left(\frac{2379989}{93312}-\frac{5\pi^2}{54}\zeta_3-\frac{3581}{648}\zeta_3-\frac{59}{60}\zeta_5+\frac{9269\pi^2}{15552}-\frac{145\pi^4}{10368}\right)\epsilon^2\Bigg]\Bigg\} \\
&+\mathcal{O}(\epsilon^3)\ ,
\end{aligned}
\tag{6.19}
$$

$$
\begin{aligned}
F_g^{(2)} \;=\; & N^2 \Bigg[ \frac{1}{2\epsilon^4} + \frac{77}{24\epsilon^3} + \frac{1}{\epsilon^2}\left(\frac{175}{72} - \frac{\pi^2}{24}\right) \\
& + \frac{1}{\epsilon}\left(-\frac{119}{54} - \frac{25}{12}\zeta_3 - \frac{11\pi^2}{144}\right) + \left(\frac{8237}{648} - \frac{33}{4}\zeta_3 + \frac{67\pi^2}{144} - \frac{7\pi^4}{240}\right) \\
& + \left(\frac{200969}{3888} + \frac{23\pi^2}{72}\zeta_3 - \frac{1139}{108}\zeta_3 + \frac{71}{20}\zeta_5 + \frac{53\pi^2}{108} - \frac{1111\pi^4}{8640}\right)\epsilon \\
& + \Bigg(\frac{4082945}{23328} - \frac{11\pi^2}{216}\zeta_3 - \frac{13109}{162}\zeta_3 + \frac{901}{36}\zeta_3^2 \\
& \quad - \frac{341}{20}\zeta_5 + \frac{85\pi^2}{1296} - \frac{1943\pi^4}{8640} + \frac{257\pi^6}{6720}\Bigg)\epsilon^2 \Bigg] \\
& + N\,N_F \left[ -\frac{7}{12\epsilon^3} - \frac{13}{12\epsilon^2} + \frac{1}{\epsilon}\left(\frac{155}{216} + \frac{\pi^2}{72}\right) \right. \\
& + \left(-\frac{5905}{1296} + \frac{1}{2}\zeta_3 - \frac{5\pi^2}{72}\right) \\
& + \left(-\frac{162805}{7776} - \frac{95}{54}\zeta_3 - \frac{11\pi^2}{432} + \frac{7\pi^4}{1440}\right)\epsilon \\
& \left. + \left(-\frac{3663205}{46656} + \frac{31\pi^2}{108}\zeta_3 + \frac{274}{81}\zeta_3 - \frac{9}{10}\zeta_5 + \frac{883\pi^2}{2592} - \frac{73\pi^4}{2592}\right)\epsilon^2 \right] \\
& + \frac{N_F}{N}\left[ -\frac{1}{8\epsilon} + \left(\frac{67}{48} - \zeta_3\right) + \left(\frac{2027}{288} - \frac{23}{6}\zeta_3 - \frac{7\pi^2}{144} - \frac{\pi^4}{54}\right)\epsilon \right. \\
& \left. + \left(\frac{47491}{1728} + \frac{5\pi^2}{18}\zeta_3 - \frac{281}{18}\zeta_3 - 4\zeta_5 - \frac{209\pi^2}{864} - \frac{23\pi^4}{324}\right)\epsilon^2 \right] + N_F^2\,\frac{1}{9\epsilon^2} \\
& + \mathcal{O}(\epsilon^3)\,.
\end{aligned}
\tag{6.20}
$$

## 6.3 Three loop master integral

We applied the new features of `HypExp` to the computation of a three-loop massless the master integral

$a_T =$ 

After Feynman parametrization, this integral reads

$$\begin{aligned}
A_T &= \mathcal{N}\Gamma(1-\epsilon)\Gamma(3\epsilon)\int\limits_0^1 du\,dt\,dz\,dy\,dr \\
&\times\ D^{-3\epsilon}(1-r)^{-3\epsilon}(1-t)^{-\epsilon}(1-y)^{\epsilon}(1-z)^{1-2\epsilon}r^{-\epsilon}z^{-3\epsilon} \\
&\times\ \Bigg(1+r\Big((1-z)zD^2+(1-y)(1-z)tD \\
&\qquad +(1-u)(1-y)^2(1-z)t^2u-1\Big)\Bigg)^{4\epsilon-2} \qquad (6.21)
\end{aligned}$$

with

$$D = 1-(1-y)(1-(1-t)(1-u)u), \quad \text{and} \quad \mathcal{N} = \frac{(4\pi)^{3\epsilon-6}}{\Gamma(1-\epsilon)^3}\left(-q^2\right)^{-3\epsilon} \qquad (6.22)$$

After numerous variable changes we get

$$\begin{aligned}
A_T &= -\frac{\mathcal{N}2^{8\epsilon-2}\pi\Gamma(1-3\epsilon)^2\Gamma(1-\epsilon)^5\Gamma(3\epsilon)}{\epsilon\Gamma(2-4\epsilon)\Gamma\left(\frac{3}{2}-2\epsilon\right)^2} \\
&\times \int\limits_0^1 (1-s)^{-3\epsilon}s^{2\epsilon-1}\left(\frac{\Gamma(1-\epsilon)^2}{\Gamma(1-2\epsilon)}-s^{-\epsilon}\,{}_2F_1(\epsilon,-\epsilon;1-\epsilon;s)\right) \\
&\times\ {}_3F_2\left(1-3\epsilon,1-2\epsilon,1-\epsilon;2-4\epsilon,\frac{3}{2}-2\epsilon;-\frac{(s-1)^2}{4s}\right) \qquad (6.23)
\end{aligned}$$

We see that we have an HF of type $3_1^0$ with one half integer parameter. We can expand each factor in $\epsilon$. The powers of $s$ and $(1-s)$ can be expressed using HPLs (and HPL weight functions)

$$\begin{aligned}
(1-s)^{-3\epsilon} &= \sum_j 3^j\epsilon^j H(^j1;s) \\
&= 1+3\epsilon H(1;s)+9\epsilon^2 H(1,1;s)+27\epsilon^3 H(1,1,1;s)+\ldots \\
(s)^{-\epsilon} &= \sum_j (-1)^j\epsilon^j H(^j1;s) \\
&= 1+2\epsilon H(0;s)+4\epsilon^2 H(0,0;s)+8\epsilon^3 H(0,0,0;s)+\ldots \\
(s)^{-1+2\epsilon} &= \frac{1}{s}\left(\sum_j 2^j\epsilon^j H(^j1;s)\right) \\
&= \frac{1}{s}\left(1+2\epsilon H(0;s)+4\epsilon^2 H(0,0;s)+8\epsilon^3 H(0,0,0;s)+\ldots\right)
\end{aligned}$$
$$(6.24)$$

The HFs can be expanded with `HypExp`. The first one has only integer parameters, the expansion will thus contain only HPLs of argument $s$. The second one has half-integer weight and will have HPLs of square root arguments

$$\sqrt{\frac{x}{x-1}}, \qquad \text{with } x = -\frac{(1-s)^2}{4s}$$

Since $s$ is in the interval $(0, 1)$, we have

$$\sqrt{\frac{x}{x-1}} = \frac{1-s}{1+s} \, ,$$

so that we can convert the HPLs of this argument into HPLs of argument $s$. The next step is to expand the product of HPLs into a sum of HPLs that we can then integrate with the integration routines of `HypExp`. The resulting HPLs are evaluated at unity. This procedure is not restricted to a specific depth of the expansion, so we could, in principle expand $A_T$ to all orders. The final result is

$$\begin{aligned}
\frac{A_T}{\mathcal{N}} &= -\frac{2\zeta(3)}{\epsilon} + \left(-\frac{7\pi^4}{180} - 18\zeta(3)\right) \\
&+ \epsilon\left(-\frac{7\pi^4}{20} - 122\zeta(3) + \frac{2}{3}\pi^2\zeta(3) - 10\zeta(5)\right) \\
&+ \epsilon^2\left(-\frac{427\pi^4}{180}\frac{163\pi^6}{7560} - 738\zeta(3) + 6\pi^2\zeta(3) + 76\zeta(3)^2 - 90\zeta(5)\right) \\
&+ \epsilon^3\Big(-\frac{287\pi^4}{20} + \frac{163\pi^6}{840} - 4202\zeta(3) + \frac{122}{3}\pi^2\zeta(3) \\
&\qquad + \frac{55}{18}\pi^4\zeta(3) + 684\zeta(3)^2 - 610\zeta(5) + \frac{445\zeta(7)}{2}\Big) \\
&+ \epsilon^4\Big(-\frac{2234}{15}\zeta_{5,3} - \frac{1117\pi^8}{70875} + \frac{4005\zeta(7)}{2} + \frac{3058}{3}\zeta(3)\zeta(5) - 3690\zeta(5) \\
&\qquad - \frac{407}{18}\pi^2\zeta(3)^2 + 4636\zeta(3)^2 + \frac{55}{2}\pi^4\zeta(3) + 246\pi^2\zeta(3) - 23058\zeta(3) \\
&\qquad \frac{7795531\pi^8}{40824000} + \frac{9943\pi^6}{7560} - \frac{14707\pi^4}{180}\Big) \\
&+ \mathcal{O}\left(\epsilon^5\right)
\end{aligned} \tag{6.25}$$

We remark that this result factorises into the following homogeneous sum where the power of $\epsilon$ grows with the transcendentality of the coefficient.

$$\frac{1}{(1-5\epsilon)(1-4\epsilon)\epsilon}$$
$$\times \Bigg[ -2\zeta(3) - \epsilon\frac{7\pi^4}{180} + \epsilon^2\left(\frac{2}{3}\pi^2\zeta(3) - 10\zeta(5)\right)$$
$$+\epsilon^3\left(\frac{163\pi^6}{7560} + 76\zeta(3)^2\right) + \epsilon^4\left(\frac{55}{18}\pi^4\zeta(3) + \frac{445\zeta(7)}{2}\right)$$
$$+\epsilon^5\left(-\frac{2234}{15}\zeta_{5,3} - \frac{1117\pi^8}{70875} + \frac{3058}{3}\zeta(3)\zeta(5) - \frac{407}{18}\pi^2\zeta(3)^2 + \frac{7795531\pi^8}{40824000}\right)\Bigg]$$
$$+\mathcal{O}(\epsilon^6) \tag{6.26}$$

## 6.4 Conclusions and outlook

In this section, we presented the computation of the two-loop quark and gluon form factors to all orders in the dimensional regularization parameter $\epsilon$. The principal ingredient to this calculation is the two-loop crossed triangle graph $A_6$, for which we computed an exact expression in terms of generalized hypergeometric functions of unit argument, which can be expanded to any desired order in $\epsilon$ using the `HypExp`-package.

An immediate application of the form factors derived here is the extraction of the complete set of infrared pole terms of the genuine three-loop quark form factor. This has been done in ref. [28].

The two-loop vertex master integrals feature as subtopologies in the reduction of the three-loop form factor contributions, appearing if one of the three loops is disconnected from the others by pinching the connecting propagators. In this case, their evaluation to $\mathcal{O}(\epsilon^2)$ is required.

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# Chapter 7

# The $qq$ real contribution to the NNLO Corrections to top pair production

## 7.1 Introduction

The top quark is by far the heaviest of the Standard Model (SM) quarks, it is so heavy that it decays before it hadronizes. This makes it to a very special tool for testing the SM and its extensions. Since its discovery at Tevatron in 1995 [1–4], anomalies in its production and decay have been searched for. The top pair kinematical distributions (e.g. invariant mass spectrum, transverse momentum distribution, etc.) can contain the first hints towards new physics. Unfortunately, the low number of top events at Tevatron seriously limits the significance of observations of top properties. At LHC, the number of top events will be very large, so that much more precise measurements can be made.

The top decays into a $b$ quark and a $W$ boson, which subsequently decay either hadronically or semi-leptonically. The experimental signature contains therefore two $b$ jets, in addition to four jets or two jets and one lepton and missing energy or two leptons and missing energy from the decays of the two $W$ bosons. These signatures can be a background to many other SM and new physics processes, like Higgs production. A good understanding of the top pair production thus improves the precision of many other important measurements.

Top pair production measured at Tevatron has an error of the order of 10%, for this accuracy, NLO theoretical predictions are sufficient. At the LHC however, the precision of the measurements will be significantly increased, due to the much higher statistics and improved $b$-tagging. Therefore the theoretical predictions have to be improved to NNLO accuracy, in order to match the experimental precision.

The LO top pair production cross section has been known since 1977 [5].

The QCD NLO order computation of the cross section for top pair production was completed in refs. [6, 7]. Electroweak and mixed EW-QCD corrections were calculated in refs. [8–12]. The cross section for top production with one jet was calculated in 1980 [13] and some contributions to its NLO QCD corrections have been calculated [14].

The task of the NNLO correction to top pair production at a hadron collider is very challenging. The tasks to accomplish are

a) two-loop virtual corrections

b) real-one-loop virtual interference corrections

c) double-real corrections

Up to now, none of these tasks have been completed.

In this chapter we will present the first step in the direction of the completion of task c). We will consider only one partonic channel, namely $qq' \to qq't\bar{t}$. This channel is suitable as a testing ground for new techniques, since the number of underlying processes is small. It is the first process where the antenna formalism [15] for initial states (see chapter 5) at NNLO order has been tested.

## 7.2 Tree level

We consider the process

$$q(p_1) + q'(p_2) \longrightarrow q(p_3) + q'(p_4) + t(p_5) + \bar{t}(p_6),$$

the quarks $q$ and $q'$ are massless whereas the top quark has mass $m_t$. We consider the two quarks to be of different flavor, so that there are no crossed diagrams. The 7 Feynman diagrams contributing to the process $qq' \to t\bar{t}$ are listed in figure 7.2. The tree level partonic cross section is then given by

$$d\sigma = \mathrm{d}\phi(p_3, p_4, p_5, p_6; p_1, p_2) \frac{1}{4N^2} |\mathcal{M}(p_1, ..., p_6)|^2 J_m^{(n)}(...; p_5, p_6) \qquad (7.1)$$

where $J_m^{(n)}(...,; p_5, p_6)$ is the function that constructs a $m$-jet observable from $n$ massless momenta. We wrote the dependence of $J$ on $p_5$ and $p_6$ explicitly, although they do not contribute to the production of jets.

The contribution of this partonic channel to the hadronic cross section is then given by

$$d\sigma_{qq}^{\mathrm{hadr}} = \int \frac{d\xi_1}{\xi_1} \frac{d\xi_2}{\xi_2} f_{q/1}(\xi_1) f_{q/2}(\xi_2) d\sigma(\xi_1 H_1, \xi_2 H_2, p_3, ..., p_6) \qquad (7.2)$$

where $H_1$ and $H_2$ are the momenta of the colliding hadrons and $f_{q/1}$, $f_{q/2}$ are the parton density functions of a quark in the hadron $H_{1,2}$.

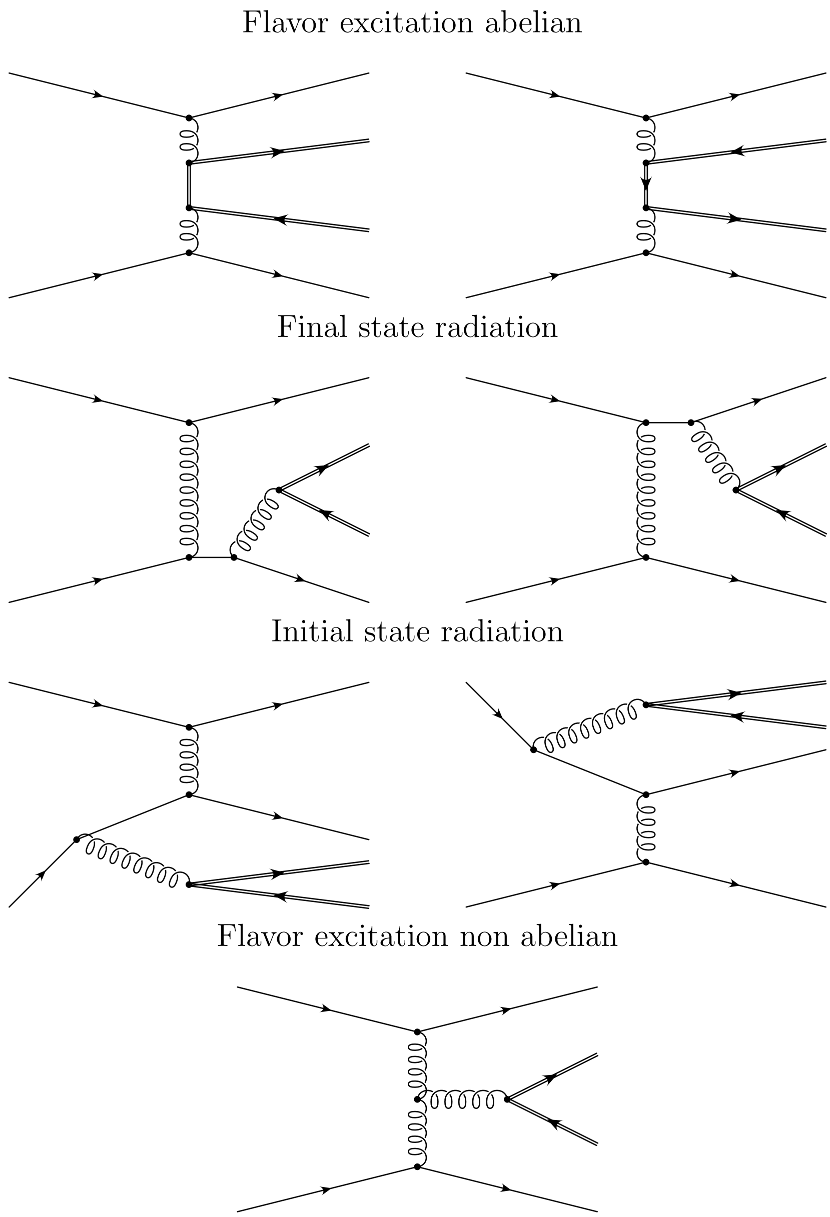



Figure 7.1: Feynman diagrams for the tree level process $qq' \to qq't\bar{t}$. Single lines are light quarks, double lines represent heavy quarks.

## 7.3 NLO contribution to $qq \to t\bar{t} + jet$

For the real correction to the partonic process $qq \to t\bar{t}+1j$ we need a subtraction term

$$d\sigma^S_{\text{NLO}}$$

that encompasses all the single soft and collinear singularities of the tree level matrix element square (7.1), but which is still easy enough to be integrated analytically for canceling the divergences coming from the virtual contribution. Given this subtraction term, the integration of the difference

$$\int \mathrm{d}\phi(p_3, p_4, p_5, p_6; p_1, p_2)\left(d\sigma - d\sigma^S_{\text{NLO}}\right) \tag{7.3}$$

over the 4 particle phasepace is finite. Using the antenna formalism described in chapter 5 the subtraction term is given by

$$\begin{aligned}
\mathrm{d}\sigma^S_{\text{NLO}} = & \\
& \frac{1}{4N^2} E_{qq',q}(p_1, p_2; p_3)(4N(N^2-1)) \\
& \times \frac{1}{4N(N^2-1)} |\mathcal{M}(gq \to qt\bar{t})|^2(\tilde{p}_{13}, \tilde{p}_2; p_3, p_5, p_6) J_1^{(1)}(p_4; p_5, p_6) \\
+ \; & E_{qq',q}(p_2, p_1; p_4)(4N(N^2-1)) \\
& \times \frac{1}{4N(N^2-1)} |\mathcal{M}(gq \to qt\bar{t})|^2(\tilde{p}_{24}, \tilde{p}_1; p_3, p_5, p_6) J_1^{(1)}(p_3; p_5, p_6) \\
= \; & \frac{N^2-1}{N} E_{qq',q}(p_1, p_2; p_3) d\tilde{\sigma}(\tilde{p}_{13}, \tilde{p}_2; p_3, p_5, p_6) J_1^{(1)}(p_4; p_5, p_6) \\
+ \; & \frac{N^2-1}{N} E_{qq',q}(p_2, p_1; p_4) \mathrm{d}\hat{\sigma}(\tilde{p}_{24}, \tilde{p}_1; p_3, p_5, p_6) J_1^{(1)}(p_3; p_5, p_6)
\end{aligned} \tag{7.4}$$

where $\mathrm{d}\tilde{\sigma}$ is the spin and colour averaged reduced matrix element

$$\mathrm{d}\tilde{\sigma} = \frac{1}{4N(N^2-1)} \left|\mathcal{M}(gq \to qt\bar{t})\right|^2 \tag{7.5}$$

and $E_{qq',q}$ is the quark gluon antenna function

$$E_{qq',q}(p_1, p_2; p_3) = \frac{s_{12}^2 - s_{12}s_{13} + (s_{13} + s_{23})s_{23}}{s_{13}(s_{12} + s_{13} + s_{23})} \tag{7.6}$$

introduced in Chapter 5. The momenta $\tilde{p}_{12}$, $\tilde{p}_{24}$, $\tilde{p}_1$, $\tilde{p}_2$ are on-shell redefined momenta built according the the mapping described in Section 5.5.2. The integrated antenna function used to cancel the poles in the pdfs reads

$$\begin{aligned}
\mathrm{d}\sigma^S = & \\
& -\frac{\alpha_S}{2\pi\epsilon} C_F \int \frac{\mathrm{d}x}{x} p_{gq}^{(0)}(x) \mathrm{d}\tilde{\sigma}(xp_1, p_2) \\
& -\frac{\alpha_S}{2\pi\epsilon} C_F \int \frac{\mathrm{d}x}{x} p_{gq}^{(0)}(x) \mathrm{d}\tilde{\sigma}(p_1, xp_2)
\end{aligned} \tag{7.7}$$

## 7.4 NNLO contribution to $qq \to t\bar{t} + 0jet$

For the real correction to the partonic process $qq \to t\bar{t}+0j$ we need a subtraction term

$$d\sigma^{S}_{\rm NNLO}$$

that encompasses all the soft and collinear singularities of the tree level matrix element square (7.1). In the case of the $qq$ induced contribution, there is only a double collinear contribution, since the quarks can not become soft. This subtraction term must however be easy enough to be integrated analytically for canceling the divergences coming from the virtual contribution. With such a subtraction term, the integral of the difference

$$\int \mathrm{d}\phi(p_3,p_4,p_5,p_6;p_1,p_2)\left(d\sigma - d\sigma^{S}_{\rm NNLO}\right) \tag{7.8}$$

over the 4 particle phasepace is finite. Using the antenna formalism described in chapter 5 the subtraction term is composed of three contributions

$$\begin{aligned}
&\mathrm{d}\sigma^{S,a}_{\rm NNLO} = \\
&\qquad \frac{1}{4N^2} E_{qq',q}(p_1,p_2;p_3)|\mathcal{M}(gq\to qt\bar{t})|^2(\tilde{p}_{13},\tilde{p}_2;p_4)J_0^{(1)}(p_4) \\
&\quad + \frac{1}{4N^2} E_{qq',q}(p_2,p_1;p_4)|\mathcal{M}(gq\to qt\bar{t})|^2(\tilde{p}_{24},\tilde{p}_1;p_3)J_0^{(1)}(p_3) \\
&\mathrm{d}\sigma^{S,b}_{\rm NNLO} = \\
&\quad - \frac{1}{4N^2} E_{qq',q}(p_1,p_2;p_3)G_{gq,q}(\tilde{p}_{13},\tilde{p}_2;p_4)|\mathcal{M}(gg\to t\bar{t})|^2(\tilde{p}_{\tilde{1}3,4},\tilde{p}_{\tilde{2},4})J_0^{(1)}(p_4) \\
&\quad - \frac{1}{4N^2} E_{qq',q}(p_2,p_1;p_4)G_{gq,q}(\tilde{p}_{24},\tilde{p}_1;p_3)|\mathcal{M}(gg\to t\bar{t})|^2(\tilde{p}_{\tilde{2}4,3},\tilde{p}_{\tilde{1},3})J_0^{(1)}(p_3) \\
&\mathrm{d}\sigma^{S,c}_{\rm NNLO} = \\
&\quad + \frac{1}{4N^2} H_{qq',qq'}(p_1,p_2;p_3,p_4)|\mathcal{M}(gg\to t\bar{t})|^2(\tilde{p}_{13},\tilde{p}_{24})J_0^{(2)}(p_3,p_4)
\end{aligned} \tag{7.9}$$

where $G_{gq,q}$ and $H_{qq',qq'}$ are the gluon-gluon antenna functions

$$G_{gq,q}(p_1,p_2;p_3) = \frac{s_{12}^2+s_{23}^2}{s_{123}^2 s_{13}} \tag{7.10}$$

$$\begin{aligned}
H_{qq',qq'}(p_1,p_2;p_3,p_4) &= \frac{2}{s_{1234}^2} \\
&+\frac{2(s_{14}s_{23}-s_{12}s_{34})^2}{s_{1234}^2 s_{13}^2 s_{24}^2} + \frac{s_{12}^2 - 2s_{34}s_{12} + s_{14}^2 + s_{23}^2 + s_{34}^2 - 2s_{14}s_{23}}{s_{1234}^2 s_{13} s_{24}}\,.
\end{aligned} \tag{7.11}$$

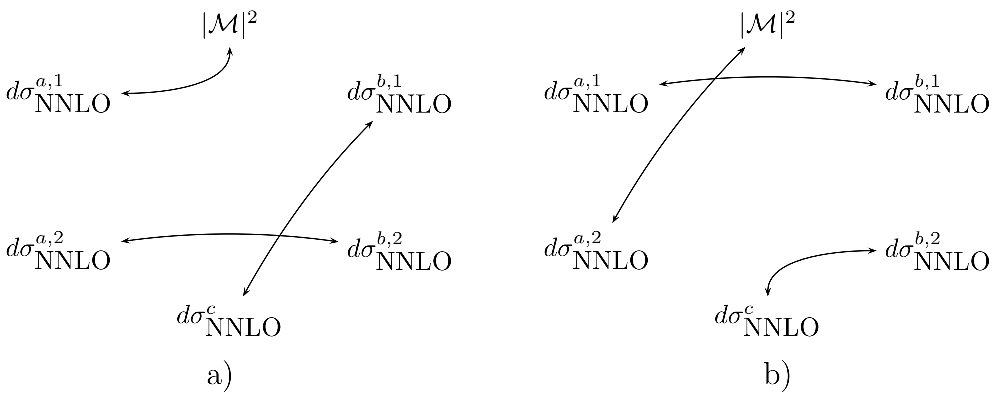



Figure 7.2: Cancellation patterns for the single collinear limit a) $s_{13} \to 0$ and b) $s_{24} \to 0$

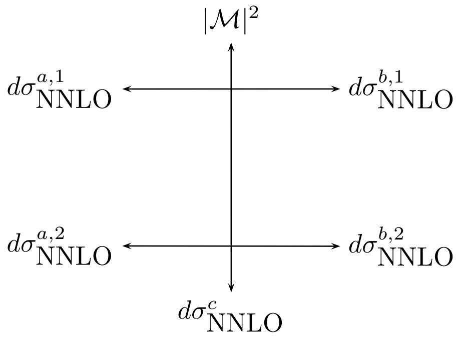



Figure 7.3: Cancellation patterns for the double collinear limit $s_{13} \to 0$ and $s_{24} \to 0$

The contribution $d\sigma^{S,c}_{\text{NNLO}}$ subtracts the double collinear limit of the matrix element. The contribution $d\sigma^{S,a}_{\text{NNLO}}$ subtracts the single collinear limits (i.e. when only one of the invariants $s_{13}$ or $s_{24}$ vanishes). The contribution $d\sigma^{S,b}_{\text{NNLO}}$ compensates both for the double collinear limits of $d\sigma^{S,a}_{\text{NNLO}}$ and the single-collinear limits of the contribution $d\sigma^{S,c}_{\text{NNLO}}$. The cancellation patterns are illustrated in the figures 7.2 and 7.3.

## 7.5 Phase space parametrisation

For the numerical implementation of the finite difference (7.8) we need to conveniently parameterize the four-particle phase space. There are many different possibilities [16]. One convenient representation is through invariants, since it is the form in which the matrix elements are expressed. In this chapter, we derive the representation of the relevant phase spaces in terms of invariants, along with improvements for their numerical implementation in a Monte Carlo integration routine.

### 7.5.1 Parameterization through invariants

In this section, we derive the parameterization of the three- and four-particle phase space appropriate to top pair production in terms of invariant scalar products.

**Three particle phase space**

The three particle phase-space element is given in $d = 4$ dimensions by

$$\mathrm{d}Q_3 = \frac{1}{(2\pi)^9}\frac{\mathrm{d}\vec{p}_1\mathrm{d}\vec{p}_2\mathrm{d}\vec{p}_3}{8E_1E_2E_3}(2\pi)^4\delta(Q - E_1 - E_2 - E_3)\delta^3(\vec{p}_1 + \vec{p}_2 + \vec{p}_3)\,. \tag{7.12}$$

We first use the $\vec{p}_3$ integration to absorb the last $\delta$-function. For the $p_2$ integration we use the results (7.64) of Appendix 7.A with

$$\vec{a} = \vec{k}_2, \qquad \vec{v} = \vec{p}_2, \qquad \vec{r} = \vec{p}_1\,,$$

we get

$$\mathrm{d}\vec{p}_2 = 2d|p_2|\,|p_2|\frac{d(\vec{k}_2\cdot\vec{p}_2)d(\vec{p}_2\cdot\vec{p}_1)}{\det|\vec{k}_2,\vec{p}_1,\vec{p}_2|}\,. \tag{7.13}$$

The integration over $\vec{p}_1\cdot\vec{p}_2$ can be used to cancel the energy $\delta$-function since

$$\begin{aligned} E_3^2 = \vec{p}_3^{\,2} + m_3^2 &= (\vec{p}_1+\vec{p}_2)^2 + m_3^2 = 2(\vec{p}_1\cdot\vec{p}_2) + \vec{p}_1^{\,2} + \vec{p}_2^{\,2} + m_3^2\,, \\ d(\vec{p}_1\cdot\vec{p}_2) &= E_3 dE_3\,, \end{aligned} \tag{7.14}$$

so that the phase-space measure becomes for massless $p_2$

$$\mathrm{d}Q_3 = \frac{1}{4(2\pi)^5}\frac{\mathrm{d}\vec{p}_1}{E_1}\mathrm{d}E_2\frac{d(\vec{k}_2\cdot\vec{p}_2)}{\det|\vec{k}_2,\vec{p}_1,\vec{p}_2|}\,. \tag{7.15}$$

Using the property $\det|a,b,c,c+d| = \det|a,b,c,d|$ and $Q = p_1+p_2+p_3+p_4$ we can transform the determinant in the denominator

$$\begin{aligned} \det|k_1,k_2,p_1,p_2| &= \frac{Q}{2}|\vec{k}_2,\vec{p}_1,\vec{p}_2| - \frac{Q}{2}|\vec{k}_1,\vec{p}_1,\vec{p}_2| + E_1|\vec{k}_1,\vec{k}_2,\vec{p}_2| - E_2|\vec{k}_1,\vec{k}_2,\vec{p}_2| \\ &= Q|\vec{k}_2,\vec{p}_1,\vec{p}_2|, \end{aligned} \tag{7.16}$$

where we used the shorthand notation

$$\det|\vec{a},\vec{b},\vec{c}| \equiv |\vec{a},\vec{b},\vec{c}|$$

The $\vec{p}_1$ integration is the easiest one. We choose polar coordinates with $z$ axis along $\vec{k}_1$. The azimuthal integration is trivial, as $\phi$ only represents the absolute orientation of $\vec{p}_1$ around the beam axis. We have:

$$\mathrm{d}\vec{p}_1 = 2\pi|\vec{p}_1|^2\mathrm{d}|p_1|\mathrm{d}\cos\psi_1. \tag{7.17}$$

We replace the $\psi_1$ integration by an integration over $k_1 \cdot p_1$:

$$d(k_1 \cdot p_1) = -d(\vec{k}_1 \cdot p_1) = -\frac{Q}{2}|\vec{p}_1|\mathrm{d}\cos\psi_1\,, \tag{7.18}$$

putting the results together yields:

$$\int \mathrm{d}Q_3 = \frac{1}{2(2\pi)^4}\int \mathrm{d}E_1 dE_2 \frac{d(\vec{k}_1 \cdot \vec{p}_1)d(\vec{k}_2 \cdot \vec{p}_2)}{\det|k_1, k_2, p_1, p_2|}\,. \tag{7.19}$$

With the identity

$$QE_i = (k_1 + k_2) \cdot p_i = (p_1 + p_2 + p_3)p_i \tag{7.20}$$

we can transform the remaining $\mathrm{d}E$ integrations into integrations over $(p_i \cdot p_j)$

$$dE_1 = \frac{d(p_1 \cdot p_3)}{Q}, \qquad dE_2 = \frac{d(p_1 \cdot p_2)}{Q}\,, \tag{7.21}$$

so that we finally get

$$\int \mathrm{d}Q_3 = \frac{1}{2^5(2\pi)^4 Q^2}\int \mathrm{d}s_1 ds_2 \frac{ds_{12}ds_{13}}{\det|k_1, k_2, p_1, p_2|}\,, \tag{7.22}$$

with

$$s_1 = (k_1 - p_1)^2, \qquad s_2 = (k_2 - p_2)^2\,.$$

**Four-particle phase space**

The four-particle phase-space element is given in $d = 4$ dimensions by

$$\begin{aligned}\mathrm{d}Q_4 = &\frac{1}{(2\pi)^{12}}\frac{\mathrm{d}\vec{p}_1\mathrm{d}\vec{p}_2\mathrm{d}\vec{p}_3\mathrm{d}\vec{p}_4}{16E_1E_2E_3E_4}\\ &\times(2\pi)^4\delta(Q - E_1 - E_2 - E_3 - E_4)\delta^3(\vec{p}_1 + \vec{p}_2 + \vec{p}_3 + \vec{p}_4)\,.\end{aligned} \tag{7.23}$$

We first use the $\vec{p}_4$ integration to absorb the last $\delta$-function. We introduce polar coordinates for $\vec{p}_3$ with $z$ axis along $\vec{p}_1 + \vec{p}_2$ and $x$ axis in the plane spanned by $\vec{p}_1$ and $\vec{p}_2$. We have then

$$\frac{\mathrm{d}\vec{p}_3}{2E_3} = \frac{1}{2}|p_3|\mathrm{d}E_3\mathrm{d}\phi\mathrm{d}\cos\Theta, \tag{7.24}$$

with $\Theta$ the angle between $\vec{p}_1 + \vec{p}_2$ and $\vec{p}_3$ and $\phi$ the azimuthal angle. The $\mathrm{d}\cos\Theta$ integration cancels the first $\delta$-function of (7.23). Since

$$\begin{aligned}E_4^2 &= \vec{p}_4^{\,2} + m_4^2 = (\vec{p}_1 + \vec{p}_2)^2 + \vec{p}_3^{\,2} + 2\vec{p}_3 \cdot (\vec{p}_1 + \vec{p}_2)\\ &= (\vec{p}_1 + \vec{p}_2)^2 + m_3^2 + 2|\vec{p}_3||\vec{p}_1 + \vec{p}_2|\cos\Theta,\end{aligned} \tag{7.25}$$

we get:

$$\frac{\mathrm{d}\vec{p}_3}{2E_3}\delta(E - E_1 - E_2 - E_3 - E_4) = \frac{E_4}{2|\vec{p}_1 + \vec{p}_2|}\mathrm{d}E_3\mathrm{d}\phi\,, \tag{7.26}$$

so that the phase-space measure becomes

$$\mathrm{d}Q_4 = \frac{\mathrm{d}\vec{p}_1\mathrm{d}\vec{p}_2}{16E_1E_2}dE_3\frac{1}{|\vec{p}_1 + \vec{p}_2|}d\phi\,. \tag{7.27}$$

For the $\phi$ integration, we use (7.63) with

$$\vec{a} = \vec{p}_1 + \vec{p}_2, \qquad \vec{r} = \vec{p}_1, \qquad \vec{v} = \vec{p}_3$$

and get

$$\mathrm{d}Q_4 = \frac{1}{16(2\pi)^8}\frac{\mathrm{d}\vec{p}_1\mathrm{d}\vec{p}_2}{E_1E_2}dE_3\frac{2d(\vec{p}_1\cdot\vec{p}_3)}{\det|\vec{p}_1 + \vec{p}_2, p_1, p_3|}\,. \tag{7.28}$$

Using the property $\det|a, b, c, c + d| = \det|a, b, c, d|$ and $Q = p_1 + p_2 + p_3 + p_4$ we can transform the determinant in the denominator

$$\begin{aligned}\det|p_1, p_2, p_3, p_4| &= E_1|\vec{p}_2, \vec{p}_3, \vec{p}_4| - E_2|\vec{p}_1, \vec{p}_3, \vec{p}_4| + E_3|\vec{p}_1, \vec{p}_2, \vec{p}_4| - E_4|\vec{p}_1, \vec{p}_2, \vec{p}_3| \\ &= -Q|\vec{p}_1, \vec{p}_2, \vec{p}_3| = Q|\vec{p}_2, \vec{p}_1, \vec{p}_3| = Q|p_1 + p_2, \vec{p}_1, \vec{p}_3|\,,\end{aligned} \tag{7.29}$$

For the $\vec{p}_2$ integration we use (7.64) with

$$\vec{a} = \vec{k}_2 + \vec{p}_2, \qquad \vec{r} = \vec{p}_1, \qquad \vec{v} = \vec{p}_2\,,$$

where $k_1$ and $k_2$ are the momenta of the two incoming particles. We get

$$\mathrm{d}Q_4 = \frac{\mathrm{d}\vec{p}_1}{16E_1}dE_2\frac{2d(\vec{p}_1\cdot\vec{p}_2)d(\vec{p}_2\cdot\vec{k}_2)}{\det|\vec{k}_2, \vec{p}_1, \vec{p}_2|}dE_3\frac{-2Qd(p_1\cdot p_3)}{\det|p_1, p_2, p_3, p_4|}\,. \tag{7.30}$$

The denominator can be simplified as follows

$$\begin{aligned}\det|k_1, k_2, p_1, p_2| &= \frac{Q}{2}|\vec{k}_2, \vec{p}_1, \vec{p}_2| - \frac{Q}{2}|\vec{k}_1, \vec{p}_1, \vec{p}_2| + E_1|\vec{k}_1, \vec{k}_2, \vec{p}_2| - E_2|\vec{k}_1, \vec{k}_2, \vec{p}_2| \\ &= Q|\vec{k}_2, \vec{p}_1, \vec{p}_2|\,,\end{aligned} \tag{7.31}$$

since in the cms we have $\vec{k}_1 = -\vec{k}_2$. The $\vec{p}_1$ integration is the easiest one. We choose polar coordinates with $z$ axis along $\vec{k}_1$. The azimuthal integration is trivial, as $\phi$ only represents the absolute orientation of $\vec{p}_1$ around the beam axis. We have:

$$\mathrm{d}\vec{p}_1 = 2\pi|\vec{p}_1|^2\mathrm{d}|p_1|\mathrm{d}\cos\psi_1. \tag{7.32}$$

We replace the $\psi_1$ integration by an integration over $k_1 \cdot p_1$:

$$d(k_1 \cdot p_1) = -d(\vec{k}_1 \cdot \vec{p}_1) = -\frac{Q}{2}|\vec{p}_1| \mathrm{d}\cos\psi_1 \,. \tag{7.33}$$

Putting the results together yields:

$$\int \mathrm{d}Q_4 = \frac{4}{16(2\pi)^8} \int 4\pi Q \mathrm{d}E_1 \mathrm{d}E_2 \mathrm{d}E_3 \frac{\mathrm{d}(k_1 \cdot p_1)\mathrm{d}(k_2 \cdot p_2)\mathrm{d}(p_1 \cdot p_2)\mathrm{d}(p_1 \cdot p_3)}{\det|p_1, p_2, p_3, p_4| \ \det|k_1, k_2, p_1, p_2|} . \tag{7.34}$$

Using the identity

$$QE_i = (k_1 + k_2) \cdot p_i = (p_1 + p_2 + p_3 + p_4)p_i \,, \tag{7.35}$$

we can transform the remaining d$E$ integrations into integration over $(p_i \cdot p_j)$

$$dE_1 = \frac{d(p_1 \cdot p_4)}{Q}, \qquad dE_2 = \frac{d(p_2 \cdot p_4)}{Q}, \qquad dE_3 = \frac{d(p_2 \cdot p_3)}{Q} \,. \tag{7.36}$$

So that we finally get

$$\begin{aligned} \int \mathrm{d}Q_4 &= \frac{4}{8(2\pi)^7 Q^2} \\ &\times \int \frac{\mathrm{d}(k_1 \cdot p_1)\mathrm{d}(k_2 \cdot p_2)\mathrm{d}(p_1 \cdot p_2)\mathrm{d}(p_1 \cdot p_3)\mathrm{d}(p_1 \cdot p_4)\mathrm{d}(p_2 \cdot p_3)\mathrm{d}(p_2 \cdot p_4)}{\det|p_1, p_2, p_3, p_4| \ \det|k_1, k_2, p_1, p_2|} \\ &= \frac{1}{2^8(2\pi)^7 Q^2} \int \frac{\mathrm{d}s_1 \mathrm{d}s_2 \mathrm{d}s_{12} \mathrm{d}s_{13} \mathrm{d}s_{14} \mathrm{d}s_{23} \mathrm{d}s_{24}}{\det|p_1, p_2, p_3, p_4| \ \det|k_1, k_2, p_1, p_2|}, \end{aligned} \tag{7.37}$$

with

$$s_1 = (k_1 - p_1)^2, \qquad s_2 = (k_2 - p_2)^2 \,.$$

### 7.5.2 Parameterization for Monte Carlo integration

For multidimensional integration over a large number of dimensions, using the usual one-dimensional numerical method for each dimension recursively is very inefficient and badly convergent. A much better method is the so-called Monte Carlo integration. In this method, points in multidimensional phase space are chosen randomly and the value of the function to be evaluated is accumulated. For a reasonably well-behaved function, the results obtained with this method converge much better than with recursive one-dimensional methods.

Monte Carlo integration can be improved by adapting the random sampling to favor either regions where the integrand is large, or where its variance is large. This can be either automatically by the Monte Carlo program, or can be done by the user of this program, since he is supposed to know more about the integrand he feeds to the program than the program itself.

In this section we describe a solution for improving the Monte Carlo integration over the four-particle phase space.

### Variance reduction

We consider the integral

$$I = \int_{x_-}^{x_+} f(x)dx \tag{7.38}$$

that we want to integrate using a Monte Carlo integration method. Since the statistical error of the Monte Carlo integration is proportional to the variance of the function $f$, the integration will be most convergent when $f$ is constant. To optimize the integration, we can perform a change of integration variable that would make the integrand look more flat. Suppose we know a function $g(x)$ that approximates the integrand $f(x)$, that is the function

$$\frac{f(x)}{g(x)}$$

is more flat than $f(x)$ and suppose that this function is however simple enough to be integrated analytically, that is we know its primitive

$$G(x) = \int^{x} dx'\, g(x')\,.$$

If we change the integration variable in (7.38) according to

$$t = G(x), \qquad x = G^{-1}(t), \qquad dt = g(x)dx\,, \tag{7.39}$$

we get the desired result

$$I = \int_{x_-}^{x_+} \frac{f(x)}{g(x)} g(x)dx = \int_{G(x_-)}^{G(x_+)} \frac{f(x(t))}{g(x(t))}dt\,. \tag{7.40}$$

We can also normalize the variable $t$ to lie in the interval $(0,1)$ by defining

$$r = \frac{G(x) - G(x_-)}{G(x_+) - G(x_-)}\,. \tag{7.41}$$

The integration becomes

$$I = \int_{x_-}^{x_+} \frac{f(x)}{g(x)} g(x)dx = G(x_+) - G(x_-) \int_0^1 \frac{f(x(r))}{g(x(r))}dr \tag{7.42}$$

with

$$x(r) = G^{-1}\left(G(x_-) + r\Delta G\right), \qquad \Delta G = G(x_+) - G(x_-)\,. \tag{7.43}$$

This integration will be more convergent, since the variance of $f/g$ is smaller than that of $f$. We illustrate the method with a simple example. Let us consider

$$I = \int_{x_{\min}}^{1} \frac{1}{x} dx, \qquad 0 < x_{\min} < 1\,. \tag{7.44}$$

this integral gets its major contribution from the region near $x = x_{\min}$ if $x_{\min}$ is small. The variance of the function on the interval $(x_{\min}, 1)$ is given by

$$\sigma = \int_{x_{\min}}^{1} dx' \left( \frac{1}{x'} - I \right)^2 = \frac{(1 - x_{\min})^2 - \log^2 x_{\min}}{(1 - x_{\min}) x_{\min}}\,, \tag{7.45}$$

which can become arbitrarily large for small values of $x_{\min}$. To reduce the variance of the function to be integrated, we should find a function $g$ that approximates the integrand. In this simple example we can take the function itself to be the approximation. We make the variable change

$$y = \log x, \qquad x = e^y, \qquad dy = x dx\,, \tag{7.46}$$

and we get for $I$

$$I = \int_{x_{\min}}^{1} \frac{1}{x} dx = \int_{\log x_{\min}}^{0} 1 dy\,. \tag{7.47}$$

Since the integrand is constant, the variance is zero (so we successfully reduced the variance of the integration...). The same variable change can be performed for integrands of the form

$$I = \int_{x_{\min}}^{x_{\max}} \frac{f(x)}{x} dx\,, \tag{7.48}$$

we get then

$$I = \int_{x_{\min}}^{x_{\max}} \frac{f(x)}{x} dx = \int_{\log x_{\min}}^{\log x_{\max}} f(e^y) dy\,, \tag{7.49}$$

which has a better variance if $f$ is flatter than $f(x)/x$.

### Variable change for the four-particle phase space

For the integration of a distribution over the four-particle phase space using the invariants parameterization described in section 7.5.1, we remark that expressed in the invariants, the phase-space density $\phi(\{s\})$ itself is not very well-behaved. The two determinants in the denominator of (7.37)

$$\det|p_1,p_2,p_3,p_4| \qquad \text{and} \qquad \det|k_1,k_2,p_1,p_2|$$

vanish at the border of the phase space. Unfortunately, most often, the main contributions to many observables are located precisely there. In addition, the regions where subtraction terms apply are, per definition, on the neighborhood of the edges of phase space. In terms of one of the integration variable $s$ in the determinant, we have for the phase-space measure

$$\phi(\{s\}) \sim \frac{F(s)}{\sqrt{as^2+bs+c}}\,. \tag{7.50}$$

The limits of the integration are the values for which the square root vanishes. We will redefine the integration variable (and thus the phase-space density), so that the integrand is effectively only $f(s)$. This integrand might still be bad-behaved, but with this variable change, the singularities due to the Gram determinant (which are commom to all distributions integrated over the four-particle phase space) are regulated. We follow the lines of the previous section 7.5.2 with

$$I = \int_{s_{\min}}^{s_{\max}} \frac{F(s)}{\sqrt{a^2(s_{\max}-s))(s-s_{\min})}}\,, \tag{7.51}$$

with $a$ a positive coefficient. Here we have the freedom to choose the invariant in the Gram determinant to be $s$. We define

$$g(s) = \frac{1}{\sqrt{(s_{\max}-s)(s-s_{\min})}}\,, \tag{7.52}$$

with primitive

$$G(s) = \int_{s_{\min}}^{s} g(s')ds' = \frac{\pi}{2} - \arctan\left(\frac{s_{\min}+s_{\max}-2s}{2\sqrt{(s_{\max}-s)(s-s_{\min})}}\right)\,. \tag{7.53}$$

According to section 7.5.2, we define the new integration variable $r$

$$r = \frac{1}{\pi}\left(\frac{\pi}{2} - \arctan\left(\frac{s_{\min}+s_{\max}-2s}{2\sqrt{(s_{\max}-s)(s-s_{\min})}}\right)\right) \tag{7.54}$$

which has the desired property

$$dr = \frac{1}{\pi}\frac{1}{\sqrt{(s_{\max}-s)(s-s_{\min})}}ds\,. \tag{7.55}$$

The variable $s$ is given by inverting (7.54)

$$s = s_{\min} + (s_{\max}-s_{\min})\cos(\pi r)\,. \tag{7.56}$$

The integral (7.51) becomes

$$I = \int_{s_{\min}}^{s_{\max}} \frac{F(s)}{\sqrt{a^2(s_{\max}-s))(s-s_{\min})}} = \frac{1}{a}\int_0^1 F(s)\,. \tag{7.57}$$

We are not yet finished, since the coefficient $a$ is given by

$$\begin{aligned} a^2 &= \frac{1}{16}(s_{12}+s_{13}-m_t^2)^2 && \text{for } \det|p_1,p_2,p_3,p_4| \\ a^2 &= \frac{1}{4}(E_1^2 Q) && \text{for } \det|k_1,k_2,p_1,p_2| \end{aligned} \tag{7.58}$$

with $Q=(k_1+k_2)^2$ and $E_1$ the energy of particle $p_1$ if we choose

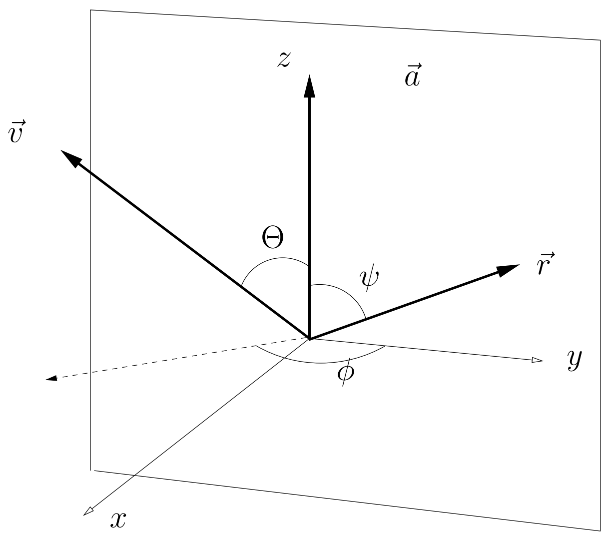
$$\begin{aligned} s &= (p_2+p_4)^2 && \text{for } \det|p_1,p_2,p_3,p_4| \\ s &= (k_2+p_2)^2 && \text{for } \det|k_1,k_2,p_1,p_2|. \end{aligned} \tag{7.59}$$

The values of $a$ can be small, so we should use equation (7.49) to flatten the density function.

## 7.A Angular integration as a function of invariants

We first consider three vectors $\vec{a}$, $\vec{r}$ and $\vec{v}$. We set the coordinate system such that

$$\vec{a} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \vec{r} = \begin{pmatrix} 0 \\ \sin\psi \\ \cos\psi \end{pmatrix}, \quad \vec{v} = \begin{pmatrix} \sin\Theta\sin\phi \\ \sin\Theta\cos\phi \\ \cos\Theta \end{pmatrix}$$



In this system we have

$$\cos\Theta_{\vec{v}\vec{r}} = \frac{\vec{v}\cdot\vec{r}}{|\vec{v}||\vec{r}|} = \sin\psi\sin\Theta\cos\phi + \cos\psi\cos\Theta \tag{7.60}$$

Considering the determinant $\det[\vec{a},\vec{r},\vec{v}]$ we find

$$\begin{aligned} \det[\vec{a},\vec{r},\vec{v}] &= \vec{a}\cdot(\vec{r}\times\vec{v}) && (7.61)\\ &= -|\vec{a}||\vec{r}||\vec{v}|\sin\Theta\sin\phi\sin\psi && (7.62)\end{aligned}$$

so that we have for fixed $|\vec{v}|$ and $|\vec{r}|$

$$\begin{aligned} \mathrm{d}(\vec{v}\cdot\vec{r}) &= |\vec{v}||\vec{r}|\mathrm{d}\cos\Theta_{\vec{v}\vec{r}}\\ &= -|\vec{v}||\vec{r}|\sin\Theta\sin\psi\sin\phi\mathrm{d}\phi\\ \Rightarrow \mathrm{d}\phi &= \frac{|\vec{a}|\mathrm{d}(\vec{v}\cdot\vec{r})}{\det[\vec{a},\vec{r},\vec{v}]} && (7.63)\end{aligned}$$

Furthermore we have

$$\vec{a}\cdot\vec{v} = |\vec{a}||\vec{v}|\cos\Theta \quad \Rightarrow \quad \mathrm{d}\cos\Theta = \frac{\mathrm{d}(\vec{a}\cdot\vec{v})}{|\vec{a}||\vec{v}|}$$

so that we finally get

$$\int \mathrm{d}^3\vec{v} = \int \mathrm{d}|\vec{v}|\,|\vec{v}|^2\mathrm{d}\cos\Theta\mathrm{d}\phi = 2\int \mathrm{d}|\vec{v}|\,|\vec{v}|\frac{\mathrm{d}(\vec{v}\cdot\vec{a})\mathrm{d}(\vec{v}\cdot\vec{r})}{\det[\vec{a},\vec{r},\vec{v}]} \tag{7.64}$$

The factor 2 accounts for the fact that one value of $\vec{v}\cdot\vec{r}$ corresponds two values or $\phi$, namely $\phi$ and $2\pi-\phi$. The last step of the above equation can only be done if the integrand is symmetric under this symmetry, which is the case when, for example the integrand is represented through scalar products.

# 7.B Analytical phase-space volume

In this section we present analytical results for the volumes for the phase spaces described in section 7.5.1. These analytical expressions can be used to test the integration routines.

## 7.B.1 Two-particle phase space

The two-particle phase space for identical masses is given by

$$dQ_2 = \frac{1}{2^2(2\pi)^{2d-2}}\int \frac{d^{d-1}\vec{p}_1}{E_1}\frac{d^{d-1}\vec{p}_2}{E_2}(2\pi)^d\delta(Q-p_1-p_2) \tag{7.65}$$

We work in the center of mass frame of $Q$ so that $E \equiv E_1 = E_2$ and $\vec{p}_1 = -\vec{p}_2$. We have

$$\begin{aligned} dQ_2 &= \frac{1}{4(2\pi)^{d-2}} \int \frac{|p_1| dE_1}{E_2} \mathrm{d}\Omega \delta(Q - 2E_1) \\ &= \frac{|\vec{p}|}{E} \frac{1}{8(2\pi)^{d-2}} \int d\Omega \qquad (7.66) \\ &= \frac{V(d-1)}{8(2\pi)^{d-2}} \frac{\sqrt{Q^2 - 4m^2}}{Q} \qquad (7.67) \end{aligned}$$

### 7.B.2 Three-particle phase space

We now consider the $1 \to 3$ phase space with one massive particle ($p_3$). The phase space is given by

$$\begin{aligned} dQ_3 &= \frac{1}{(2\pi)^{3d-3}} \int \frac{d^{d-1}\vec{p}_1}{2E_1} \frac{d^{d-1}\vec{p}_2}{2E_2} \frac{d^{d-1}\vec{p}_3}{2E_3} (2\pi)^d \delta^d(Q - p_1 - p_2 - p_3) \\ &= \frac{1}{8(2\pi)^{2d-3}} \frac{d^{d-1}\vec{p}_1}{E_1} \frac{d^{d-1}\vec{p}_2}{E_2} \delta(Q - E_1 - E_2 - E_3) \qquad (7.68) \end{aligned}$$

Since

$$\begin{aligned} E_3^2 &= \vec{p}_3^{\,2} + m_3^2 = (\vec{p}_1 + \vec{p}_2)^2 + m_3^2 = \vec{p}_1^{\,2} + 2\vec{p}_1 \cdot \vec{p}_2 \cos\Theta_{12} + \vec{p}_2^{\,2} + m_3^2 \\ d^{d-1}p_2 &= |p_2|^{d-3} d|p_2| d\cos\Theta_{12} d\Omega_{d-2} \qquad (7.69) \end{aligned}$$

$$\begin{aligned} dQ_3 &= \frac{1}{8(2\pi)^{2d-3}} \int \frac{d^{d-1}p_1}{E_1} \frac{dE_2}{|\vec{p}_1|} E_2^{d-4} \, d\Omega_{d-2} \\ &= \frac{V(d-2)V(d-1)}{8(2\pi)^{2d-3}} \int dE_1 dE_2 (E_1 E_2)^{d-4} \end{aligned}$$

From the conditions

$$-1 < \cos\Theta_{12} = \frac{(Q - E_1 - E_2)^2 - E_1^2 - E_2^2 - m_3^2}{2E_1 E_2} < 1$$

we can derive the limits for the $E_2$ integration as a function of $E_1$.

$$\begin{aligned} E_2^{\min} &= \frac{Q^2 - 2E_1 Q - m_3^2}{2Q} \\ E_2^{\max} &= \frac{Q^2 - 2E_1 Q - m_3^2}{2(Q - 2E_1)} \qquad (7.70) \end{aligned}$$

The requirement that the energy $E_1$ must be positive imposes

$$E_1^{\max} = \frac{Q^2 - m_3^2}{2Q}$$

We can perform the integration in $d = 4$ dimensions and find

$$R_3(Q, m_3) \equiv \int dQ_3 1 = \frac{1}{32\pi^3} \frac{Q^4 + 2m_3^2 Q^2 \log\left(\frac{m_3^2}{Q^2}\right) - m_3^4}{8Q^2}$$

We recover the known massless result,

$$R_3(Q) = \frac{Q^2}{256\pi^3},$$

by setting $m_3 \to 0$.

### 7.B.3 Four-particle phase space

We now consider the four-particle phase space with two massless particles and two massive particle of the same mass $m_t$. We can use the result of the sections 7.B.1 and 7.B.2 in the following way. We multiply

$$1 = \int d^d k \delta^d(k - p_3 - p_4) \int dm^2 \delta(m^2 - k^2)$$

in the expression for the four-particle phase space,

$$\int dQ_4 = \frac{1}{(2\pi)^{4(d-1)}} \int \frac{d^{d-1}p_1}{2E_1} \frac{d^{d-1}p_2}{2E_2} \frac{d^{d-1}p_3}{2E_3} \frac{d^{d-1}p_4}{2E_4} (2\pi)^d \delta^d(Q - p_1 - p_2 - p_3 - p_4)$$

so that we get

$$\begin{aligned} \int dQ_4 &= \frac{1}{16(2\pi)^{3d-4)}} \int \frac{d^{d-1}p_1}{E_1} \frac{d^{d-1}p_2}{E_2} \int dm^2 \frac{d^{d-1}k}{2E_k} \delta^d(Q - p_1 - p_2 - k) \\ &\quad \times \int \frac{d^{d-1}p_3}{E_3} \frac{d^{d-1}p_4}{E_4} \delta^d(k - p_3 - p_4) \\ &= \frac{1}{2\pi} \int dm^2 dQ_3(Q; p_2, p_2, k) dQ_2(k; p_3, p_4), \end{aligned} \tag{7.71}$$

where now the momentum $k$ has mass $k^2 = m^2$. Since we are interested in the phase-space volume, there are no correlations between the two phase spaces $dQ_2$ and $dQ_3$, the phase space $dQ_2(k; p_3, p_4)$ only depend on $k$ through $k^2 = m^2$. We then get (in $d = 4$ dimensions)

$$\begin{aligned} \int dQ_4 &= \frac{1}{2\pi} \int dm^2 dQ_3(Q; p_2, p_2, k) dQ_2(k; p_3, p_4) \\ &= \frac{1}{2\pi} \frac{1}{2^5\pi^3} \frac{1}{8\pi} \int dm^2 \frac{Q^4 + 2m^2 Q^2 \log\left(\frac{m^2}{Q^2}\right) - m^4}{8Q^2} \sqrt{1 - 4\frac{m_t^2}{m^2}} \end{aligned} \tag{7.72}$$

We define the variables

$$\lambda = \frac{m^2}{Q^2} \to dm^2 = Q^2 d\lambda, \qquad \mu = \frac{4m_t^2}{Q^2}$$

With these definitions the phase-space volume looks

$$\int dQ_4 \;=\; \frac{Q^4}{2^{12}\pi^5} \int d\lambda (1 + 2\lambda \log\lambda - \lambda^2) \sqrt{1 - \frac{\mu}{\lambda}} \tag{7.73}$$

We now make the change of variable

$$\omega = \sqrt{1 - \frac{\mu}{\lambda}}, \qquad \lambda = \frac{\mu}{1-\omega^2}, \qquad d\lambda = \frac{2\omega\mu}{(1-\omega^2)^2}$$

and finally get

$$\int dQ_4 = \frac{2\mu^2 Q^4}{2^{12}\pi^5} \int_0^{\sqrt{1-\mu}} d\omega \left[ \frac{\omega^2}{(1-\omega^2)^2} + \frac{\mu}{1-\omega^3} \left( H_-(\omega) + H_0(\omega) \right) - \mu^2 \frac{\omega^2}{(1-\omega^2)^4} \right] \tag{7.74}$$

where we converted the logarithms into HPLs. In this form, we can use the same integration routines for HPLs used for the expansion of hypergeometric functions described in chapter 3. The result reads

$$\begin{aligned} R_4(Q, m_t) \;=\; & -\frac{1}{48} Q^4 \\ \times\; & \left[ 12\mu^2 \left( \mathrm{Li}_2\left(\frac{1+\sqrt{1-\mu}}{2}\right) - \mathrm{Li}_2\left(\frac{1-\sqrt{1-\mu}}{2}\right) \right) \right. \\ & +3\mu \left( (\mu-4)(\mu+2) + 2\mu \log\left(\frac{4}{\mu}\right) \right) \log\left(\frac{1-\sqrt{1-\mu}}{1+\sqrt{1-\mu}}\right) \\ & \left. -2\sqrt{1-\mu}(4 + 20\mu + 3\mu^2) \right] \end{aligned} \tag{7.75}$$

## 7.C Angular integration in $d$ dimensions

To perform the integration over the the orientations in $d-1$ space dimensions, we introduce spherical coordinates for the $d-1$ space dimensions.

$$x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{d-2} \\ x_{d-1} \end{pmatrix} = r \begin{pmatrix} \sin\Theta_{d-2} \sin\Theta_{d-3} \ldots \sin\Theta_2 \sin\Theta_1 \\ \sin\Theta_{d-2} \sin\Theta_{d-3} \ldots \sin\Theta_2 \cos\Theta_1 \\ \sin\Theta_{d-2} \sin\Theta_{d-3} \ldots \cos\Theta_2 \\ \vdots \\ \sin\Theta_{d-2} \cos\Theta_{d-3} \\ \cos\Theta_{d-2} \end{pmatrix} \tag{7.76}$$

The integration over the $d-1$-dimensional space is given in term of these coordinates by:

$$\int \mathrm{d}\vec{x} = \int_0^\infty \mathrm{d}r\, r^{d-2} \int_0^{2\pi} \mathrm{d}\Theta_1 \\ \times \int_0^\pi \mathrm{d}\Theta_2 \sin\Theta_2 \ldots \int_0^\pi \mathrm{d}\Theta_j \sin^{j-1}\Theta_j \ldots \int_0^\pi \mathrm{d}\Theta_{d-2} \sin^{d-3}\Theta_{d-2} \quad (7.77)$$

The integration over $\mathrm{d}\Omega_n$ gives the surface of the unit sphere in $n$ space-dimensions:

$$\int \mathrm{d}\Omega_n = \frac{2\pi^{n/2}}{\Gamma(\frac{n}{2})} = V(n) \quad (7.78)$$

The values of $V(n)$ for some integers $n$ are listed below:

| $n$ | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| $V(n)$ | 2 | $2\pi$ | $4\pi$ | $2\pi^2$ | $\frac{8\pi^2}{3}$ |

We consider the integration of products of scalar products

$$\int \mathrm{d}\Omega_{d-1}\, (k\cdot p_1)\,(k\cdot p_2)\ldots(k\cdot p_m)$$

over the $d-1$-dimensional orientations.

$$\int \mathrm{d}\Omega_{d-1} = \int_0^{2\pi} \mathrm{d}\Theta_1 \int_0^\pi \mathrm{d}\Theta_2 \sin\Theta_2 \ldots \int_0^\pi \mathrm{d}\Theta_{d-2} \sin^{d-3}\Theta_{d-2} \quad (7.79)$$

There are two possible strategies

- take the three "physical" dimensions to be 1,2,3. We take the fixed vectors $p_i$ to lie all in the space spanned by these three directions.

  This means that the scalar products between $k$ and the $p_i$'s will be the product of the "3-dimensional" scalar products and a factor containing $d-3$ sine

  $$k\cdot p_i \to (k\cdot p_i)_3 \sin\Theta_3 \ldots \sin\Theta_{d-2}$$

  Here one perform the integration in "physical" 3-dimensions and multiply by a factor corresponding to the integration of this sine over the $d-1$

orientation space

$$
\begin{aligned}
&\int \mathrm{d}\Omega_{d-1}(k)(\sin\Theta_3 \ldots \sin\Theta_{d-2})^m \prod_m (k\cdot p_i)_3 = \\
&= \int \underbrace{\mathrm{d}\Theta_1 \sin\Theta_2 \mathrm{d}\Theta_2}_{\mathrm{d}\Omega_3} \prod_m (k\cdot p_i)_3 \\
&\quad \times \int \sin^{2+m}\Theta_3 \mathrm{d}\Theta_3 \sin^{3+m}\Theta_4 \mathrm{d}\Theta_4 \ldots \sin^{d-3+m}\Theta_{d-2}\mathrm{d}\Theta_{d-2} \\
&= \int \mathrm{d}\Omega_3 \prod_m (k\cdot p_i)_3 \frac{V(d+m-1)}{V(d-1)} \\
&= \frac{\pi^{\frac{d-4}{2}}\Gamma\left(\frac{3+m}{2}\right)}{\Gamma\left(\frac{d-1+m}{2}\right)} \int \mathrm{d}\Omega_3 \prod_m (k\cdot p_i)_3
\end{aligned}
$$

- take the three "physical" dimensions to be $d-1$,$d-2$,$d-3$. We take the fixed vectors $p_i$ to lie all in the space spanned by these three directions.

  Here the scalar products are like in 3 dimensions, but the price to pay is that the Jacobian has now sine to the power $d-2$,$d-3$ and $d-4$.

  The method is in this case the following. One first expresses all scalar products as function of $\cos\Theta$ and $\sin^2\Theta$. The terms proportional to an odd power of $\cos\Theta$ vanish due to symmetry. Then one uses

$$
\int_0^\pi \sin^n\Theta = \frac{V(n+2)}{V(n+1)}
$$

  To treat the remaining sine:

$$
\begin{aligned}
\sin^m\Theta \quad \rightarrow \quad & \int \sin^m\Theta \sin^{d-3-j}\Theta_{d-2+j} \\
&= \int \sin^{m+d-3-j}\Theta_{d-2+j} = \frac{V(d-1+m-j)}{V(d-2+m-j)}
\end{aligned}
\tag{7.80}
$$

  This method is the most applicable if there are not only scalar products, but also denominators. It is easier to integrate a simple scalar product (without the sine tail) in the denominator times a sine to the power $d$ than a denominator containing the sine tail which would have to be integrated iteratively $d$ times.

## 7.C.1 Applications

Let us consider the integration of $f(\psi_1, \psi_2, \psi_3)$, a function of three angles over the $d-1$-dimensional space (corresponding to the $d$-dim space-time). Putting $\Theta_{d-2} = \psi_1$, $\Theta_{d-3} = \psi_2$, $\Theta_{d-4} = \psi_3$ in 7.79 we get

$$\begin{aligned}\int \mathrm{d}\Omega_{d-1} f(\psi_1, \psi_2, \psi_3) &= \int_0^{2\pi} \mathrm{d}\Theta_1 \int_0^{\pi} \mathrm{d}\Theta_2 \sin\Theta_2 \ldots \int_0^{\pi} \mathrm{d}\Theta_{d-5} \sin^{d-6}\Theta_{d-5} \\ &\quad\times \int_0^{\pi} \mathrm{d}\psi_3 \sin^{d-5}\psi_3 \int_0^{\pi} \mathrm{d}\psi_2 \sin^{d-4}\psi_2 \int_0^{\pi} \mathrm{d}\psi_1 \sin^{d-3}\psi_1 f(\psi_1, \psi_2, \psi_3) \\ &= V(d-4) \int_0^{\pi} \mathrm{d}\psi_3 \sin^{d-5}\psi_3 \int_0^{\pi} \mathrm{d}\psi_2 \sin^{d-4}\psi_2 \int_0^{\pi} \mathrm{d}\psi_1 \sin^{d-3}\psi_1 f(\psi_1, \psi_2, \psi_3)\end{aligned}$$

Assuming that the function $f$ contains only integer powers of sines and cosines of $\psi_{1,2,3}$, we will have to treat integrals of the form

$$\int_0^{\pi} \sin^n\psi \, \cos^m\psi \qquad , \quad m \in \mathbb{Z}$$

First we split the integration in two pieces, one from 0 to $\pi/2$ and the other from $\pi/2$ to $\pi$. We can write the second integration also as an integration over the first interval by performing the change of variable $\psi \to \pi - \psi$. This changes the sign of the cos and leaves the sin unchanged. This means that the integral vanishes for $m$ odd. For $m$ even we have

$$\begin{aligned}\int_0^{\pi} \sin^n\psi \, \cos^m\psi &= 2\int_0^{\frac{\pi}{2}} \sin^n\psi \, \cos^m\psi \\ &= 2\int_0^1 \frac{\mathrm{d}t}{\sqrt{1-t^2}} t^n \left(\sqrt{1-t^2}\right)^m = \int_0^1 \mathrm{d}u u^{-\frac{1}{2}} u^{\frac{n}{2}} \sqrt{1-u}^{m-1} = \frac{\Gamma(\frac{n+1}{2})\Gamma(\frac{m+1}{2})}{\Gamma(1+\frac{n+m}{2})}\end{aligned}$$

So that we get

$$\boxed{\int_0^{\pi} \sin^n\psi \, \cos^m\psi = \begin{cases} 0 & m \text{ odd} \\ \dfrac{\Gamma(\frac{n+1}{2})\Gamma(\frac{m+1}{2})}{\Gamma(1+\frac{n+m}{2})} & m \text{ even} \end{cases}}$$

The previous example applies only if there are no denominators containing functions of the angles $\psi_{1,2,3}$. The next example has a denominator dependent on one angle. We start by computing

$$\int_0^{\pi} \frac{\sin^n\psi \, \cos^m\psi}{a^2 - b^2\cos^2\psi_1} \mathrm{d}\psi, \qquad m \in \mathbb{N}$$

We need to keep the power $m$ integer valued since we want to make use of the reflection identity

$$cos\theta = -\cos(\pi - \theta)$$

We use the substitution

$$y = \cos^2\psi, \quad \mathrm{d}y = 2\cos\psi\sin\psi, \quad \sin\psi = \sqrt{1-y}, \quad \cos\psi = \sqrt{y}$$

and get for $m$ even

$$\begin{aligned}
\int_0^\pi \frac{\sin^n\psi\,\cos^m\psi}{a^2 - b^2\cos^2\psi_1}\mathrm{d}\psi &= 2\int_0^1 \frac{\frac{1}{2}\sin^{n-1}\cos^{m-1}\psi\mathrm{d}y}{a^2 - b^2 y} \\
= \int_0^1 \frac{\sqrt{y}^{n-1}\sqrt{1-y}^{m-1}}{a^2\left(1 - y\frac{b^2}{a^2}\right)} &= \frac{1}{a^2}\frac{\Gamma(\frac{n+1}{2})\Gamma(\frac{m+1}{2})}{\Gamma(1+\frac{n+m}{2})}{}_2F_1\left(1, \frac{m+1}{2}, \frac{n+m}{2}+1; \frac{b^2}{a^2}\right)
\end{aligned}$$

we can now treat the more general case

$$\begin{aligned}
\int_0^\pi \frac{\sin^n\psi\,\cos^m\psi}{(a - b\cos\psi_1)}\mathrm{d}\psi &= \int_0^{\pi/2} \frac{\sin^n\psi\,\cos^m\psi}{(a - b\cos\psi_1)}\mathrm{d}\psi + \int_{\pi/2}^\pi \frac{\sin^n\psi\,\cos^m\psi}{(a - b\cos\psi_1)}\mathrm{d}\psi \\
= &\int_0^{\pi/2} \frac{\sin^n\psi\,\cos^m\psi}{(a - b\cos\psi_1)}\mathrm{d}\psi + \int_{\pi/2}^\pi \frac{\sin^n\psi\,(-1)^m\cos^m(\pi-\psi)}{(a + b\cos\psi)}\mathrm{d}\psi \\
= &\int_0^{\pi/2} \frac{\sin^n\psi\,\cos^m\psi}{(a - b\cos\psi)}\mathrm{d}\psi + (-1)^m\int_0^{\pi/2} \frac{\sin^n\psi'\,\cos^m(\psi')}{(a + b\cos\psi')}\mathrm{d}\psi' \\
= &\int_0^{\pi/2} \frac{\sin^n\psi\,\cos^m\psi}{(a^2 - b^2\cos\psi)}\left(a + b\cos\psi) + (-1)^m(a - b\cos\psi)\right)\mathrm{d}\psi \\
= &\int_0^{\pi/2} \mathrm{d}\psi\frac{\sin^n\psi}{(a^2 - b^2\cos\psi)}\left\{\begin{array}{ll} 2a\cos^m\psi & m\,\text{even} \\ 2b\cos^{m+1}\psi & m\,\text{odd}\end{array}\right.
\end{aligned} \tag{7.81}$$

using the above result we get

$$\int_0^\pi \frac{\sin^n\psi\,\cos^m\psi}{(a-b\cos\psi_1)}\mathrm{d}\psi =$$
$$\begin{cases} \dfrac{1}{a}\dfrac{\Gamma(\frac{n+1}{2})\Gamma(\frac{m+1}{2})}{\Gamma(1+\frac{n+m}{2})}{}_2F_1\left(1,\dfrac{m+1}{2},\dfrac{n+m}{2}+1;\dfrac{b^2}{a^2}\right) & m\,\text{even} \\ \dfrac{b}{a^2}\dfrac{\Gamma(\frac{n+1}{2})\Gamma(\frac{m}{2}+1)}{\Gamma(1+\frac{n+m+1}{2})}{}_2F_1\left(1,\dfrac{m}{2}+1,\dfrac{n+m+1}{2}+1;\dfrac{b^2}{a^2}\right) & m\,\text{odd} \end{cases} \tag{7.82}$$

This generalizes easily to the case of integer power $k$ of the denominator

$$\int_0^\pi \frac{\sin^n\psi\,\cos^m\psi}{(a-b\cos\psi_1)^k}$$

one expands the bracket

$$\big((a+b\cos\psi)^k+(-1)^m(a-b\cos\psi)^k\big)$$

in the second-to-last line of 7.81

$$\int_0^\pi \frac{\sin^n\psi\,\cos^m\psi}{(a-b\cos\psi_1)^2}\mathrm{d}\psi$$
$$= \begin{cases} \quad\dfrac{1}{a^2}\dfrac{\Gamma(\frac{n+1}{2})\Gamma(\frac{m+1}{2})}{\Gamma(1+\frac{n+m}{2})}{}_2F_1\left(2,\dfrac{m+1}{2},\dfrac{n+m}{2}+1;\dfrac{b^2}{a^2}\right) & \\ \quad+\dfrac{b^2}{a^4}\dfrac{\Gamma(\frac{n+1}{2})\Gamma(\frac{m+3}{2})}{\Gamma(2+\frac{n+m}{2})}{}_2F_1\left(2,\dfrac{m+3}{2},\dfrac{n+m}{2}+2;\dfrac{b^2}{a^2}\right) & m\,\text{even} \\ \dfrac{2b}{a^3}\dfrac{\Gamma(\frac{n+1}{2})\Gamma(\frac{m}{2}+1)}{\Gamma(1+\frac{n+m+1}{2})}{}_2F_1\left(2,\dfrac{m}{2}+1,\dfrac{n+m+1}{2}+1;\dfrac{b^2}{a^2}\right) & m\ \text{odd.} \end{cases} \tag{7.83}$$

Since the cosine of powers larger one can rewritten in terms of sines, we are only interested in the results for $m=0,1$ using the above result we get

$$\int_0^\pi \frac{\sin^n\psi\,\cos^m\psi}{(a-b\cos\psi_1)}\mathrm{d}\psi = \begin{cases} \dfrac{1}{a}\dfrac{\Gamma(\frac{n+1}{2})\sqrt{\pi}}{\Gamma(1+\frac{n}{2})}{}_2F_1\left(1,\dfrac{1}{2},\dfrac{n}{2}+1;\dfrac{b^2}{a^2}\right) & m=0 \\ \dfrac{b}{a^2}\dfrac{\Gamma(\frac{n+1}{2})\sqrt{\pi}}{(n+2)\Gamma(\frac{n}{2}+1)}{}_2F_1\left(1,\dfrac{3}{2},\dfrac{n}{2}+2;\dfrac{b^2}{a^2}\right) & m=1 \end{cases} \tag{7.84}$$

similarly for the square of the denominator:

$$\int_0^\pi \frac{\sin^n\psi\ \cos^m\psi}{(a-b\cos\psi_1)^2}\mathrm{d}\psi =$$
$$\begin{cases} \dfrac{1}{a^2}\dfrac{\Gamma(\frac{n+1}{2})\sqrt{\pi}}{\Gamma(1+\frac{n}{2})}\,{}_2F_1\left(2,\dfrac{1}{2},\dfrac{n}{2}+1;\dfrac{b^2}{a^2}\right) & \\ +\dfrac{b^2}{a^4}\dfrac{\Gamma(\frac{n+1}{2})\sqrt{\pi}}{(n+2)\Gamma(\frac{n}{2}+1)}\,{}_2F_1\left(2,\dfrac{3}{2},\dfrac{n}{2}+2;\dfrac{b^2}{a^2}\right) & m=0 \\ \\ \dfrac{2b}{a^3}\dfrac{\Gamma(\frac{n+1}{2})\sqrt{\pi}}{(n+2)\Gamma(\frac{n}{2}+1)}\,{}_2F_1\left(2,\dfrac{3}{2},\dfrac{n}{2}+2;\dfrac{b^2}{a^2}\right) & m=1. \end{cases} \tag{7.85}$$

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